Unblocking of the Gamow-Teller strength in stellar electron capture on neutron-rich germanium isotopes

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We propose a new model to calculate stellar electron capture rates for neutron-rich nuclei. These nuclei are encountered in the core collapse of a massive star. Using the shell model Monte Carlo approach, we first calculate the finite temperature occupation numbers in the parent nucleus. We then use these occupation numbers as a starting point for calculations using the random phase approximation (RPA). Using the RPA approach, we calculate electron capture rates including both allowed and forbidden transitions. Such a hybrid model is particularly useful for nuclei with proton numbers Z < 40 and neutron numbers N > 40, where allowed Gamow-Teller transitions are only possible due to configuration mixing by the residual interaction and by thermal unblocking of pf-shell single-particle states. Using the even germanium isotopes $^{68-76}$ Ge as examples, we demonstrate that the configuration mixing is strong enough to unblock the Gamow-Teller transitions at all temperatures relevant to core-collapse supernovae.

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Current one-dimensional core-collapse supernova models fail to produce explosions [1,2]. A forefront area of research involves determining whether this failure is due to incorrect microphysics input or whether it implies that the explosion actually requires multidimensional effects like convection and rotation. More likely, both the microphysics and hydro-dynamical effects will play important roles in enhancing our understanding of supernovae explosions. One important aspect of microphysics that determines the fate of a core-collapse supernova is electron capture on protons and nuclei. These weak captures serve to deleptonize the core of the massive star and determine the final electron fraction, Y_e , and therefore they set the size of the homologous core.

In his review [3], Bethe described the development of theories and models of electron-capture in supernovae environments. Early models assumed that the capture takes place on free protons. This view was revised by Bethe and collaborators [4] who noted the low concentration of free protons relative to iron-group nuclei and the strong Gamow-Teller (GT) transitions for $f_{7/2}$ protons to be changed into $f_{5/2}$ neutrons. These authors concluded that electron capture during the collapse phase takes place on nuclei in the mass range A = 60 - 80. Subsequently, Fowler, Fuller, and Newman developed the formalism for stellar weak processes [5] and estimated the rates for electron capture on nuclei with A ≤ 60 (and for other weak processes) on the basis of the independent particle model and available experimental data. Recent decisive progress in nuclear modeling, coupled with computational advances, made possible reliable calculations of stellar electron capture and beta-decay rates. These rates were calculated for pf-shell nuclei in large shell-model spaces [6]. Although these improved rates lead to significant changes in the supernova progenitor models [7,8], they confirm the FFN results: electron captures in supernova progenitor models indeed take place on complex nuclei in the iron mass range.

While the iron region has been sufficiently investigated, we know that the distinct possibility exists for electron capture to occur in nuclei beyond the pf shell. Historically, this possibility has not been included in core-collapse simulations. Fuller [9] pointed out that the Pauli principle blocks Gamow-Teller transitions by neutrons if one uses the independent-particle model with Z < 40 and $N \ge 40$. In this model, the *pf* shell is completely occupied by neutrons. It was concluded that electron capture in this region once again proceeds by free protons. Modern collapse simulations still treat electron capture on the basis of the independent particle model (even reduced to a model which only considers $f_{7/2}$ and $f_{5/2}$ orbitals [10]) and also block all capture on nuclei with $N \ge 40$ [11]. In contrast, Cooperstein and Wambach noted from an investigation based on the random phase approximation [12], that electron capture on neutron-rich nuclei with protons in the pf shell and neutron number N >40 can compete with capture on free protons if one considers forbidden transitions in addition to allowed ones. They also demonstrated that at high enough temperatures, $T \sim 1.5$ MeV, Gamow-Teller transitions are thermally unblocked primarily as a result of the excitation of neutrons from the pfshell into the $g_{9/2}$ orbital. This unblocking allows GT transitions within the pf shell, which then again dominate the electron capture rates. We will argue in this Rapid Communication that electron capture on nuclei with N>40 is also dominated by GT transitions even at rather low stellar temperatures near T = 0.5 MeV. This effect occurs since configuration mixing induced by the residual interactions and thermal excitations are already strong enough to unblock the GT transitions.

We consider a stellar environment with temperature T. The total cross section for capture of an electron with energy E_e (rest mass plus kinetic) on a nucleus with charge Z and mass number A is given by

$$\sigma(E_{e},T) = \frac{G_{w}^{2}}{2\pi} \sum_{i} F(Z,E_{e}) \frac{(2J_{i}+1)e^{-E_{i}/(kT)}}{G(Z,A,T)}$$
$$\times \sum_{f,\lambda} (E_{e}-Q_{if})^{2} \frac{|\langle i|T_{\lambda}|f\rangle|^{2}}{(2J_{i}+1)}, \qquad (1)$$

where G_w is the weak-interaction coupling constant and $F(Z, E_{e})$ is the Fermi function that accounts for the Coulomb distortion of the electron wave function near the nucleus (see, for example, [6]). The sum over initial states involves a thermal average of levels, with excitation energies E_i in the parent nucleus; G(Z,A,T) is the respective partition function. Each initial state i is connected to various final states fvia multipole operators T_{λ} which were derived in [13]. These operators, in principle, depend on the momentum transfer; however, at the energies involved here, momentum transfer is small. Under these conditions, the $\lambda = 1^+$, T_{λ} operator reduces to the Gamow-Teller operator $\sigma \tau_+$ (which changes a proton into a neutron). We include the so-called quenching of the GT strength by multiplying the GT transition matrix element by the constant factor 0.7 [14,15]. The Q value for a transition between initial and final states is given by Q_{if} $= M_f - M_i + E_f - E_i = Q + E_f - E_i$, where $M_{i,f}$ are the masses of the parent and daughter nuclei and E_f is the excitation energy of the final state.

The nuclei of interest in this study are expected to contribute to the stellar electron capture rates for temperatures $T \approx 0.5 - 1.5$ MeV. At such high temperatures an explicit state-by-state evaluation of the sums in Eq. (1) is impossible with current nuclear models. As was noted and applied in [5,16], the cross section expression becomes significantly simplified assuming the Brink hypothesis. Brink conjectured that the strength distribution of the multipole operators in the daughter nucleus is the same for all initial states and shifted by the excitation energy of the initial state. By using this approximation, the sum over final states becomes independent of the initial state and the sum over the Boltzmann weights cancels the partition function. Although the shellmodel calculations of [6] in fact verify this approximation for *pf*-shell nuclei in the temperature range of interest, it cannot be naively applied to the nuclei here since the unblocking of the Gamow-Teller strength should be strongly state dependent; i.e., the probability of $g_{9/2}$ configuration mixing will increase with excitation energy. Cooperstein and Wambach accounted for this effect by a state-by-state evaluation of the cross section: they reduced the sum over initial states to the spectrum of the RPA single-particle levels. As the energy splitting between the $g_{9/2}$ orbital and the pf shell is of the order of 2-3 MeV, the thermal unblocking required quite high temperatures in [12].

At the present time, detailed shell-model calculations for neutron-rich nuclei with Z < 40 and $N \ge 40$ are feasible only for a few nuclei. Furthermore, the development of a generally reliable shell-model interaction for nuclei in this region has not yet occurred. In order to make some progress in this astrophysically important region, we therefore propose a model for the calculation of electron capture on heavy nuclei that is computationally feasible and incorporates relevant

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nuclear structure physics. We also assume the Brink hypothesis; however, we apply it to an initial state which represents the thermal average of many-body states in the parent nucleus at temperature T. We describe this thermally averaged initial state by a Slater determinant with partial occupation numbers for the relevant single-particle states. Obviously the partial occupation numbers are a function of temperature. Adopting the Brink hypothesis and describing the initial state by the representative Slater determinant with temperature-dependent occupation numbers $n_i(T)$, the electron capture cross section reduces to

$$\sigma(E_e,T) = \frac{G_w^2}{2\pi} F(Z,E_e) \sum_k (E_e - Q - \omega_k)^2 \sum_{\lambda} S_{\lambda}(\omega_k,T),$$
(2)

where ω is the excitation energy in the daughter nucleus and S_{λ} is the discrete random phase approximation (RPA) response for the multipole operator λ . In the RPA approach [21], multipole operators up to $\lambda = 2$ are considered, and the single-particle energies are taken from a standard Woods-Saxon parametrization that is very close to the values used in Ref. [12].

We obtain the thermal occupation numbers that we use in the RPA calculations from canonical shell model Monte Carlo (SMMC) [17] calculations. SMMC techniques have been demonstrated to well describe the thermal properties of nuclei [18]. For the germanium isotopes $^{68-76}$ Ge, we adopted the complete $(pfg_{9/2})$ shell-model space and used a pairing+quadrupole residual interaction [19] with parameters appropriate for this region. Two reasons guide our choice here: first, a reliable shell-model interaction for neutron-rich nuclei in this region is not yet available; second, we wish to avoid the Monte Carlo sign problem associated with using realistic interactions in SMMC [18]. By avoiding the sign problem, we are able to calculate occupation numbers with less statistical error. For our purposes, this constitutes a reasonable first attempt to incorporate the relevant many-body physics and to understand the effects of temperature and residual interaction on the Gamow-Teller strengths in neutron-rich nuclei. We adopted the single-particle energies from the KB3 interaction [20], but we artificially reduced the $f_{5/2}$ orbital by 1 MeV to simulate the effects of the $\sigma\tau$ component that is missing in our residual interaction. We assumed an energy splitting of 3 MeV between the $g_{9/2}$ and the $f_{5/2}$ orbitals.

We performed SMMC calculations for all even germanium isotopes $^{68-76}$ Ge at various temperatures between T = 0.5 MeV and 1.3 MeV. As representative examples, Figs. 1 and 2 show the calculated proton and neutron occupation numbers for the nucleus 74 Ge. In the independent particle model (IPM) the 12 valence protons completely occupy the $f_{7/2}$ and $p_{3/2}$ orbitals, while the $p_{1/2}$, $f_{5/2}$, and $g_{9/2}$ orbitals are empty. (Obviously IPM predicts the same proton occupation numbers for all germanium isotopes.) For the 22 valence neutrons, the IPM predicts a full pf shell and two neutrons occupying the $g_{9/2}$ orbital. Clearly, the IPM does not allow GT transitions for 74 Ge.

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FIG. 1. Proton occupation percentage $n_i(T)/(2j_i+1)$ in ⁷⁴Ge for the independent particle model (IPM, circles) and calculated in the SMMC approaches at T=0.5 MeV (squares) and 1.3 MeV (diamonds). The single-particle energies have been determined from a Woods-Saxon potential: -16.1 MeV ($f_{7/2}$), -11.0 MeV ($p_{3/2}$), -10.7 MeV ($f_{5/2}$), -9.0 MeV ($p_{1/2}$), and -7.0 MeV ($g_{9/2}$).

The residual interaction of the shell model distorts the naive independent particle picture significantly. Furthermore, thermal excitation of the nucleus further perturbs the single-particle occupations. Both the configuration mixing due to the residual interaction and the thermal excitations of the many-body system act to smear the Fermi surface. This physics is captured by the SMMC approach. We observe in Fig. 1 that for both temperatures the occupation of the proton $p_{3/2}$ orbital is only about half and that even the occupation of the neutron $g_{9/2}$ orbital is nearly doubled, resulting in two neutron holes in the pf shell.

Even at T=0.5 MeV, the SMMC calculation predicts $\langle n \rangle = 0.72$ protons in the $g_{9/2}$ orbital, while for the other iso-



FIG. 2. Neutron occupation percentage $n_i(T)/(2j_i+1)$ in ⁷⁴Ge for the independent particle model (IPM, circles) and calculated in the SMMC approaches at T=0.5 MeV (squares) and 1.3 MeV (diamonds). The single-particle energies have been determined from a Woods-Saxon potential: -19.1 MeV ($f_{7/2}$), -14.5 MeV ($p_{3/2}$), -13.6 MeV ($f_{5/2}$), -12.5 MeV ($p_{1/2}$), and -10.2 MeV ($g_{9/2}$).

IPM T=0.5 MeV T=1.3 MeV 2.5 [10⁻⁴²cm²] 51 -- 1– 1----- 2ь 1.0 0.5 0.0 0 5 10 15 0 5 10 15 0 5 10 15 Q-value [MeV]

....

3.0

FIG. 3. Dominating multipole contributions $\lambda = 1^+$ (solid), 1^- (long-dashed), and 2^- (dotted) for the differential capture cross section for 20 MeV electrons on ⁷⁴Ge. The calculations have been performed within the independent particle model and for temperatures T=0.5 MeV and 1.3 MeV using the hybrid SMMC/RPA model as described in the text. The *Q* value for T=0 is 5.4 MeV.

topes the average number of protons in this orbital is 0.65 (^{70}Ge) , 0.59 (^{72}Ge) , 0.52 (^{74}Ge) , and 0.48 (^{76}Ge) . For the same temperature, the SMMC studies yield 5.8 neutron holes in the pf shell for ⁶⁸Ge (compared to 4 in the IPM). As expected, the number of neutron holes is reduced in the other isotopes; we find 4.3 (⁷⁰Ge), 3.1 (⁷²Ge), 2.0 (⁷⁴Ge), and 1.1 (⁷⁶Ge). These partial occupations make possible Gamow-Teller transitions since there are neutron holes in the pf shell and protons in the $g_{9/2}$ orbital; therefore, we expect from these occupation numbers that GT transitions for electron capture are not completely blocked. Even at the rather low temperature T = 0.5 MeV, configuration mixing and thermal excitations smear the Fermi surface. This contrasts with the RPA study of Ref. [12] which found no significant unblocking. The difference between the results is that the SMMC calculations consider the thermal excitation of all many-body states, while Ref. [12] considered the thermal excitation of only the single-particle states in the model space. The unblocking that we find might be quite important. Recent presupernova evolution models imply that Y_{ρ} is ~0.44 for T =0.5 MeV [8]; this corresponds roughly to the proton-tonucleon ratio in ^{72,74}Ge.

Figure 3 shows the decomposition of the capture cross section for 20 MeV electrons on ⁷⁴Ge into the leading multipoles $\lambda = 1^+, 1^-, 2^-$. The calculation has again been performed in the IPM and in the hybrid model at T = 0.5 MeV and 1.3 MeV. As noted before [9,12], unblocking is most important for allowed transitions, although one also observes a slight redistribution of the strength for the forbidden dipole transitions. Obviously the differences are very pronounced for the GT transition. While transitions are blocked in the independent particle model Gamow-Teller, they dominate the response in the hybrid model. The two prominent peaks in the RPA response correspond to $f_{7/2} \rightarrow f_{5/2}$ and $g_{9/2}$ $\rightarrow g_{7/2}$ proton-neutron transitions. However, unblocking also allows particle-to-particle transitions between partially occupied orbitals. For some of these transitions, the energy difference between the initial and final single-particle states is



FIG. 4. Electron capture cross sections for 68,72,76 Ge calculated within the independent particle model (solid) and for temperatures T=0.5 MeV (long-dashed) and 1.3 MeV (dotted) using the hybrid SMMC/RPA model as described in the text.

negative and can even lead to unphysical, negative Q values (see Fig. 3). Fortunately these transitions do not contribute significantly to the total cross section.

Our expectations about the importance of GT unblocking are realized in the total electron capture calculations we performed using the RPA method. The results are exemplified in Fig. 4 for ⁶⁸Ge with four neutron holes even in the simple IPM, and for ^{72,76}Ge for which the IPM does not allow GT transitions. These differences are well pronounced in the IPM capture rates, showing large cross sections for ⁶⁸Ge. For ^{72,76}Ge, electron capture is mediated by forbidden transitions resulting in cross sections which are more than two orders of magnitude smaller than for ⁷⁶Ge at moderate electron energies ($E_e < 15$ MeV). Note that capture of an electron with energy E_e is more difficult on ⁷⁶Ge than on ⁷²Ge, due to the increased Q value. We also note that the IPM cross sections become clearly more similar for larger electron energies as the sensitivity to the Q value decreases and the relative importance of the forbidden transitions increases.

When we repeat the calculations for 68 Ge using the occupation numbers from the SMMC calculations, we find a rather small reduction in the capture cross section. Since GT transitions were already allowed in the IPM, the residual interaction and thermal effects are quite unimportant for this nucleus. We also note that forbidden transitions do not significantly contribute to electron capture on *pf*-shell nuclei at moderate electron energies. This confirms the assumption made in previous studies that the capture rate for *pf*-shell nuclei during the presupernova evolution can be solely de-

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termined on the basis of GT transitions.

Configuration mixing and thermal excitations unblock the GT transitions in ⁷²Ge and ⁷⁶Ge. This effect is strong enough in both nuclei to increase the capture cross section by nearly two orders of magnitude at the lowest electron energies shown in Fig. 4. Our calculations indicate that the unblocking effect is not too sensitive to increasing temperature. This is certainly of strong practical importance as it indicates that SMMC studies do not have to be performed on very fine temperature grids, and extrapolations should be quite sufficient. At higher electron energies, forbidden transitions become important since the differences between the SMMC/RPA and IPM cross sections diminish.

In summary, in the collapse phase of a supernova, electrons can be captured on very neutron-rich nuclei with protons in the pf shell (Z<40) and neutron numbers N>40. For these nuclei, Gamow-Teller transitions, which dominate electron capture on *pf*-shell nuclei during the presupernova evolution, are forbidden in the independent particle model. We have shown that this model is too simple for applications to neutron-rich isotopes, since GT transitions are unblocked by finite temperature excitations and by the mixing of occupations of the *pf* and $g_{9/2}$ orbitals induced by the residual interaction. In this paper, we propose a hybrid model in which the temperature and configuration-mixing effects are studied within the shell model Monte Carlo approach and are described by partial occupation numbers for the various single-particle orbits. Using the mean-field wave function with these corresponding partial occupancies, the electron capture cross sections are calculated with an RPA approach. We considered both allowed GT and forbidden transitions.

We applied our hybrid model to the even germanium isotopes $^{68-76}$ Ge at typical collapse temperatures $T \sim 0.5 - 1.5$ MeV. At all temperatures, the residual interaction is sufficiently strong to unblock the GT transitions which then also dominate stellar electron capture on these nuclei. However, with increasing electron energies, i.e., at larger electron chemical potentials and temperatures, forbidden transitions become increasingly important and can no longer be neglected. The present model consistently describes allowed and forbidden transitions and should thus be also applicable to such situations.

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