Nuclear Weak Rates and Detailed Balance in Stellar Conditions

G. Wendell Misch$^{1,2}$

$^1$Department of Physics and Astronomy, Shanghai Jiao Tong University, 800 Dong Chuan Road, Shanghai 200240, China; wendell@sjtu.edu, wendell.misch@gmail.com

$^2$Collaborative Innovation Center of IFSA (CICIFSA), Shanghai Jiao Tong University, China

Received 2017 January 5; revised 2017 June 7; accepted 2017 June 7; published 2017 July 18

Abstract

Detailed balance is often invoked in discussions of nuclear weak transitions in astrophysical environments. Satisfaction of detailed balance is rightly touted as a virtue of some methods of computing nuclear transition strengths, but I argue that it need not necessarily be strictly obeyed in astrophysical environments, especially when the environment is far from weak equilibrium. I present the results of shell model calculations of nuclear weak strengths in both charged-current and neutral-current channels at astrophysical temperatures, finding some violation of detailed balance. I show that a slight modification of the technique to strictly obey detailed balance has little effect on the reaction rates associated with these strengths under most conditions, though at high temperature the modified technique in fact misses some important strength. I comment on the relationship between detailed balance and weak equilibrium in astrophysical conditions.

Key words: astroparticle physics – neutrinos – nuclear reactions, nucleosynthesis, abundances – supernovae: general

1. Introduction

Weak interactions play crucial roles in the evolution of stars of all masses, influencing both the chemical evolution of their material content and the transport of energy. Main-sequence stars convert hydrogen to helium via either the p–p chain or the C–N–O cycle, both of which convert protons to neutrons via charged-current (CC) weak interactions. In stars of mass greater than $\sim 8-12 M_\odot$ (solar masses), beginning with core carbon fusion, energy and entropy are carried out of the core almost entirely by neutrinos. Initially, most of these neutrinos are produced as pairs via thermal processes in the plasma (Itoh et al. 1996; Patton et al. 2017), but as stars near collapse, nuclei play an important—and eventually dominant—role in neutrino production (Arnett 1977; Bethe et al. 1979; Odrzywolek et al. 2004; Langanke 2015; Asakura et al. 2016). Stars at the very low end of this mass region, with $M \sim 8-10 M_\odot$, may collapse due to loss of electron pressure support as nuclei in the mass range $A = 20-24$ capture electrons (Nomoto 1987; Hüdepohl et al. 2010; Martínez-Pinedo et al. 2014). More massive stars will continue nuclear fusion until silicon burning builds up an iron core that eventually collapses, producing neutrinos from a variety of nuclear sources, especially electron capture (EC) on heavier nuclei. Nuclear weak rates, particularly $\beta$-decay rates, also influence evolution in other environments; they are critical in nucleosynthesis processes through their effect on waiting points in the r-process (rapid neutron capture) and rp-process (rapid proton capture), as well as in neutron star cooling and Type Ia supernovae (Kratz et al. 1986; Kratz 1988; Lattimer et al. 1991; Page & Applegate 1992; Engel et al. 1999; Martínez-Pinedo & Langanke 1999; Sarriguren et al. 2005; Bazin et al. 2008; Mori et al. 2016). In light of the pervasive influence of nuclear weak interactions, we naturally desire the most accurate rates possible to use in models of stellar and chemical evolution.

There are six principal nuclear weak interaction processes in stellar environments—four CC reactions and two neutral-current (NC): EC, electron emission ($\beta$-decay), positron capture, positron emission, neutrino scattering, and NC de-excitation, shown schematically in Figure 1. The last of these is similar to nuclear gamma-ray emission, but instead of a photon, the nucleus emits a virtual $Z^0$ boson that decays into a neutrino–antineutrino pair. Under conditions with large neutrino fluxes, the outgoing neutrinos in the Feynman diagrams of Figure 1 can be changed to incoming, yielding the neutrino capture processes. These processes are all sensitive to the masses and structure of nuclei.

Unfortunately, nuclear properties are notoriously difficult to compute accurately, particularly at finite temperature, and nuclear weak rates and neutrino energy spectra depend sensitively on these properties. Much of the difficulty lies in the limitations of computers, because nuclei are complex many-body quantum mechanical systems that must be solved numerically. Researchers have developed numerous techniques to simplify the problem and make good approximations, which, coupled with increasing computer power, are gradually yielding more and more reliable results. Detailed balance often comes up in discussions of such approximations. It refers to the relationship between the forward and reverse transition strengths of a quantum mechanical system: the forward and reverse amplitudes from an initial state $|\psi\rangle$ to a final state $|f\rangle$ are complex conjugates. Because a realistic model must obey detailed balance, it can be invoked to simplify calculations, sparing the invoker direct computation of the reverse reaction strengths, and it also ensures that this aspect of the model is realistic.

Fuller et al. (1980, 1982a, 1982b, 1985) performed one of the earliest broad surveys of CC nuclear weak rates, considered accurate enough for use over the past few decades. Their work employed the standard of using experimentally measured nuclear energies and transition strengths where available and using approximation techniques to fill the gaps. In particular, they assumed all allowed transitions with unknown strength to have $\log (f_{\text{full}})/f_{\text{comparative}}$ values of 5: $f_{\text{full}}$ is the comparative half-life of the transition from initial nuclear state $|\psi\rangle$ to final nuclear state $|f\rangle$ and is related to the matrix elements for nuclear weak interaction (Brown et al. 1978). Then, they adapted the Brink–Axel
assumption that the Gamow–Teller resonance occurred in excited states with the same strength and same relative transition energy as in the ground state. Because they also included “back resonances,” this method obeys detailed balance, but the downsides of the technique of Fuller et al. are twofold. First, there can be significant variation in the allowed transition strengths, so the assumption of log (\( f_{\gamma} \)) = 5 for all unknown transitions holds only in an average sense. Second, the adaptation of the Brink–Axel hypothesis to weak interaction strength breaks down for initial-state excitation energies of more than a few MeV (Misch et al. 2014).

Oda et al. (1994) sought to circumvent these issues by performing large-scale shell model calculations on \( sd \)-shell nuclei (nuclei with mass numbers \( A = 17–39 \)). In their calculations, they supplemented known experimental energies and strengths with computations of the 100 lowest-lying states in each \( sd \)-shell nucleus found using the shell model. Because all 100 states are included as both initial and final states and no additional states are considered, this method obeys detailed balance, and it is effective over a broad range of conditions. However, it suffers the single biggest pitfall of shell model calculations: the model space must be restricted in order to avoid “dimensional explosion.” The Hamiltonian that must be diagonalized has, of course, dimension equal to the number of basis states, and restriction ensures the number of particle configurations (which correspond to basis states) is small enough to be computable in a reasonable time. Oda et al. used the restriction of a single valence shell (the \( sd \) shell), asserting an inert \( ^{16}O \) core and inaccessible single-particle states above the valence shell. This implies the exclusion of negative parity states, as they require excitation of particles from the core to the \( sd \) shell and/or from the \( sd \) shell to the \( fp \) shell, both of which greatly increase the model space and consequently the computational requirements. In defense of Oda et al., the missing negative parity states likely do not have a large effect on the total rates, because the lowest-lying (and hence statistically most important) states are positive parity. However, restriction to the lowest 100 nuclear states may miss some important features of states at very high energy, especially when considering neutrino spectra.

Caurier et al. (1999) and Langanke & Martínez-Pinedo (2000, 2001) performed large-scale shell model calculations on nuclei in the mass range \( A = 45–65 \), corresponding to the \( fp \) shell. But, as discussed above, shell model calculations quickly become intractable as the number of configurations grows. The configurations grow roughly exponentially with \( A \) (assuming significantly more available states than particles), so this technique is restricted to lighter nuclei unless some kind of truncation is imposed. In this case, the authors of those works considered a closed \( ^{40}Ca \) core and only computed relatively low-lying nuclear energies of a few MeV. By restricting themselves to low-lying nuclear states, they can plausibly consider only a few particles excited above the lowest-energy single-particle configuration. Another approach to truncation of the model space is Monte Carlo shell model methods, where more valence particles are allowed to occupy excited levels, but not all multiparticle configurations are included (Johnson et al. 1992; Koonin et al. 1997).

In order to approach heavier nuclei, some authors have employed the quasiparticle random-phase approximation (QRPA; Dzhioev et al. 2010, 2015; Sarriguren 2013). While this approach is satisfactory at locating the centroid of strength distributions and obeys detailed balance, numerous studies have shown it to underperform the shell model in finding the detailed nuclear structure to which weak rates are sensitive over a broad range of mass, including both the \( sd \) shell (Lauritzen 1988; Civitarese et al. 1991) and the \( fp \) shell (Auerbach et al. 1993; Zhao & Brown 1993; Cole et al. 2012). Indeed, Cole et al. (2012) found that QRPA substantially overestimated the Gamow–Teller strength relative to both the shell model and experiment, Xu et al. (2014) were better able to reproduce their experimental \( \beta \)-decay half-lives using the shell
model, and Schwengner et al. (2010) found that the shell model better reproduced experimental data for the strength and distribution of the giant dipole resonance in $^{208}$Pb. The shell model has been exceptionally successful at matching experimental observations of nuclear energy levels and weak transition strengths from nuclear ground states, as well as M1 electromagnetic transition strengths (Brown & Wildenthal 1985, 1988); the last of these can also be measured between excited states in a gamma cascade. The principal culprit in this failure of QRPA is the fact that—in contrast to the dimensional explosion that limits the utility of the shell model—QRPA uses relatively few basis states. This allows much faster calculations, but at the cost of predictive capability.

The difficulties of heavy nuclei necessitate the development of modern techniques to treat nuclear many-body problems efficiently. Considering that most nuclei in the nuclear chart are deformed, working with an appropriately deformed single-particle basis instead of a spherical basis is more computationally economical. This is because a single deformed basis state is composed of a linear combination of spherical states, but because the nucleus is deformed, the deformed state contains more realistic physical information about the nucleus. The result is that a much smaller number of deformed single-particle configurations need to be considered to accurately model the nucleus, which reduces the model space and hence the required computational power. Angular momentum is not a good quantum number in a deformed basis and needs to be restored, since nuclei do have well-defined angular momentum. By using an angular momentum projection method, these deformed single-particle states can be made to have good angular momentum, transforming them into a suitable set of basis states for a shell model (Hara & Sun 1995; Sun 2016). The projected shell model has been successful in describing many structural properties of deformed nuclei, making it a promising approach. It has not yet been broadly employed to compute CC weak interactions, but recent developments indicate that it might be very useful for just that in the near future (Gao et al. 2006; L.-J. Wang et al. 2017, in preparation).

The conclusion we must ultimately arrive at is that, as of now, we simply cannot precisely calculate nuclear weak rates (and nuclear neutrino spectra) under all conditions, so we must make decisions about what to sacrifice. This paper will make the case that among the things we can sacrifice is strict adherence to detailed balance of nuclear weak thermal strength, particularly when the environment of interest is out of weak equilibrium.

In Section 2 I define nuclear weak interaction thermal strengths and the quantity imbalance. Section 3 describes a method of producing thermal strengths from shell model calculations and shows the results for several nuclei along with associated imbalances. Section 4 defines phase-space factors, and in Section 5 I present rate calculations for $^{32}$P using two different but related methods. In Section 6, I talk about environments far from weak equilibrium and how that relates to detailed balance.

2. Thermal Strength and Imbalance

In the language of Fischer et al. (2013), detailed balance of the NC thermal strength is expressed as

$$S^{{GT3}}(T, \Delta E) = e^{\Delta E/T}S^{{GT3}}(T, -\Delta E)$$

where $T$ is the temperature and $\Delta E$ is the nuclear transition energy (final excitation energy minus initial excitation). $S^{{GT3}}$ is the NC thermal strength, given by

$$S^{{GT3}}(T, \Delta E) = \frac{1}{G(T)} \int_0^\infty dE (2J + 1) \rho(E, J) \times e^{-E/T}B^{{GT3}}(E, \Delta E)$$

where $G(T)$ is the nuclear partition function, $E$ is the initial nuclear excitation energy, $J$ is the nuclear spin, $\rho(E, J)$ is the density of nuclear states, and $B^{{GT3}}(E, \Delta E)$ is the strength for a transition from a state with energy $E$ and a transition energy of $\Delta E$.

The thermal strength on the left of Equation (1) is that of the forward reaction, and the strength on the right corresponds to the reverse reaction. In keeping with the appeal of symmetry, put the forward and reverse reactions on equal footing by rewriting Equation (1) as

$$e^{-\Delta E/T}S^{{GT3}}(T, \Delta E) = e^{\Delta E/T}S^{{GT3}}(T, -\Delta E).$$

Equation (3) has some conceptual subtleties that are worth touching on. Naturally, it applies to all NC nuclear interactions, including lepton pair emission, lepton pair absorption, and scattering. Notably, the reverse reaction thermal strength is not considered directly, but rather is mirrored about $\Delta E = 0$. The physical meaning of this is that we are comparing “up transitions” (transitions with positive $\Delta E$, where the nucleus gains energy) in the forward reaction directly with the corresponding “down transitions” (negative $\Delta E$) in the reverse reaction, and vice versa.

At finite temperature, the forward reaction will have nonzero strength for both up and down transitions (implying the same for the reverse reaction). Depending on the reactions, this might be physically absurd; NC neutrino scattering on nuclei can certainly proceed through either up or down nuclear transitions as the nucleus takes energy from or gives energy to the neutrino, but neutrino pair absorption cannot have negative nuclear transition energy, and pair emission cannot induce the nucleus to gain energy. If the reactions under consideration do not allow up (or down) transitions, then simply neglect the corresponding domain of $\Delta E$ as being unphysical. This argument also applies to CC interactions. For the sake of completeness, this discussion of thermal strength and the associated figures will contain the full domain of $\Delta E$ with no reference to a specific reaction. Note, though, that this work always considers reverse reactions with the $-\Delta E$ argument as in Equation (3); this can make confusing-looking distributions of reverse reaction strength, so keep in mind that we are in fact comparing up transitions against down transitions.

The expression for detailed balance of CC thermal strength differs slightly from that for the NC channel. We begin with the CC thermal strength for transitions from nucleus $j$ to nucleus $k$, defined analogously to the NC:

$$S^{{\pm}}_{jk}(T, Q) = \frac{1}{G_j(T)} \int_0^\infty dE_j (2J + 1) \rho_j(E_j, J_j) e^{-E_j/T}B^{{\pm}}_{jk}(E_j, Q).$$

The plus (minus) signs in the superscripts correspond to isospin-raisin (-lowering) transitions, $G_j(T)$ is the partition function of nucleus $j$, and $Q$ is the total nuclear transition energy from an initial state in nucleus $j$ with energy $E_j$ to a final...
state in nucleus \( k \) with energy \( E_k \).

\[
Q \equiv E_k + m_t - E_j - m_j.
\]

(5)

Extending the observations of Thomas (1964, 1968) and Grover & Gilat (1967) to CC interactions yields

\[
(2J + 1) \rho_k(E_i, J) B_{kk}^{\pm}(E_k, Q) = (2J + 1) \rho_k(E_k, J) B_{kk}^{\pm}(E_k, -Q).
\]

(6)

Substituting into Equation (4) and using Equation (5) to substitute \( E_k \) for \( E_j \) gives

\[
S_{kk}^{\pm}(T, Q) = \frac{1}{G_j(T)} \int_{-\infty}^{\infty} dE_k (2J + 1) \rho_k(E_k, J) \\
	imes e^{-(E_k - Q + \Delta m)/T} B_{kk}^{\pm}(E_k, -Q)
\]

(7)

where \( \Delta m \equiv m_k - m_j \). The lower limit of this integral must obviously be at least zero (even if \( Q - \Delta M < 0 \)) since nuclear excitation can never be less than zero. \( E_k = Q - \Delta m \) corresponds to \( E_j = 0 \), so any values of \( E_k < Q - \Delta m \) correspond to values of \( E_j < 0 \), which is unphysical. Interpreting this as meaning that \( B_{kk}^{\pm}(E_k < Q - \Delta m, -Q) = 0 \), simply consider the lower limit on the integral to be zero. This yields

\[
S_{kk}^{\pm}(T, Q) = \frac{1}{G_j(T)} \int_{0}^{\infty} dE_k (2J + 1) \rho_k(E_k, J) \\
	imes e^{-(E_k - Q + \Delta m)/T} B_{kk}^{\pm}(E_k, -Q)
\]

\[
= \frac{G_k(T)}{G_j(T)} e^{(Q - \Delta m)/T} S_{kk}^{\pm}(T, -Q).
\]

(8)

Rewriting to match the format of Equation (3), we at last arrive for the expression for the detailed balance of CC thermal strength:

\[
e^{-(Q - \Delta m)/2T} G_j(T) S_{kk}^{\pm}(T, Q) = e^{(Q - \Delta m)/2T} G_k(T) S_{kk}^{\pm}(T, -Q).
\]

(9)

Unlike the NC channel, this expression includes factors of each nuclear partition function because the initial and final nuclei are not identical.

Following Misch & Fuller (2016), define the imbalance \( I \) between two positive quantities \( A \) and \( B \) as

\[
I(A, B) = \frac{A - B}{A + B}.
\]

(10)

I use imbalance to compare quantities throughout this work, because it has some advantages over other traditional quantities of comparison, e.g., ratios and differences. First, imbalance is (anti)symmetric in \( A \) and \( B \). Second, it is finite if either argument is zero. Both of these qualities make it preferable to a ratio here, since many of the quantities compared in this work can be small or zero. Third, it gives a measure of relative inequality—rather than absolute inequality—making it preferable to a difference when comparing quantities of arbitrary size such as transition strengths.

Imbalance has the disadvantage of not allowing an immediate, intuitive direct comparison (e.g., \( A \) is four times as large as \( B \)). In this work, we are more concerned with trends than precise numbers, so our lack of intuition is no great hindrance. However, this lack may simply be because we are not yet used it, and perhaps intuition can be aided with a simple mechanical analog: two objects with masses \( m_1 \) and \( m_2 \) suspended under gravity on either side of a physicist’s pulley (massless, frictionless). Obviously, if the masses are equal, their acceleration will be zero, and if one mass is greater than the other, it will accelerate downward at some rate less than the acceleration of gravity \( g \) while the other accelerates upward. If one mass is much greater than the other, the acceleration will be nearly \( g \). In fact, the acceleration is always \( g \times I(m_1, m_2) \), so imbalance \( I(A, B) \) behaves precisely according to its namesake.

3. Shell Model Calculations

As discussed above, weak rates are sensitive to nuclear structure, and the shell model has been the most successful technique for reproducing experimental results. Therefore, I used the shell model code OXBASH (Brown et al. 2004) and the USDB Hamiltonian (Brown & Richter 2006) to compute nuclear energy levels and transition strengths for both CC and NC transitions in several \( sd \)-shell nuclei. As with Oda et al., I assume an inert \( ^{16}O \) core and allow only \( sd \)-shell configurations. USDB does a satisfactory job of reproducing nuclear energy levels and matrix elements for various transitions, including the channels considered here (Richter et al. 2008). However, it overpredicts the Gamow–Teller matrix elements by a factor of \( \sim 1.3 \), so I applied a uniform quenching factor of 0.6 to the strengths to bring them more in line with experiment (strength is proportional to the square of the matrix element: \( \langle \frac{1}{1.3} \rangle ^2 \approx 0.6 \)). Additionally, when specific experimental data exist, I did not rely on theoretical calculations; I computed the full spectrum of energies and strengths for each nucleus using OXBASH, then replaced theoretical values with measured values by hand. A limitation of these calculations is that they entirely neglect forbidden transitions, which can play a major role late in collapse. However, the intent of this work is to illustrate a general property of out-of-equilibrium nuclear weak interactions in stellar conditions, the conclusions of which will extend to forbidden transitions.

The modification of the Brink–Axel hypothesis proposed by Misch et al. (2014) is to include all states individually up to a cutoff energy and combine several states above the cutoff into a single high-energy average state that carries the remainder of the thermal statistical weight. This prescription is effective for computing EC and energy loss rates, but the lack of states at very high initial nuclear energy renders it unsatisfactory at producing neutrino energy spectra at very high neutrino energy. Initial states with energies above the high-energy average state must be included to see the neutrino spectrum at very high neutrino energy. Initial states with energies above the high-energy average state must be included to see the neutrino spectrum at very high neutrino energy, particularly in the NC channel where all of the neutrino energy comes from the nucleus (as opposed to the CC channel, where incoming leptons provide some of the energy). Therefore, I further modified the technique of Misch et al. (2014) and used the following approach. I considered all initial nuclear states individually up to 15 MeV. I took as lower cutoff energy and combine several states above the cutoff into a single high-energy average state that carries the remainder of the thermal statistical weight corresponding to states in its bin.

For the initial states under 15 MeV excitation (those considered individually), I computed the transition strengths
to all final states in the daughter nucleus with total energy less than 35 MeV above the ground state of the parent nucleus. For the binned initial states, I computed transition strengths to all final states below 20 MeV above the respective lower bin edge. This likely clips the tail at high transition energy of the strength distributions of the highest energy initial states, but this is mitigated in three ways. First, there is very little strength above 20 MeV transition energy. Second, the high-energy initial states are sparsely populated. Third, transitions with large, positive transition energy require incoming particles with correspondingly high energy. For CC reactions, this can only happen at an appreciable rate late in stellar core collapse when the electron Fermi energy is extremely high, and for the NC, after core bounce, when energetic neutrinos are produced. I converted the resulting strength distributions to thermal strengths according to Equations (2) and (4) and compared the forward and reverse strengths by computing their imbalance (Equation (10)); recall that distributions of reverse reaction strength are mirrored about \( Q = 0 \) so that we can compare up transitions to down transitions. I also computed the concomitant imbalance between the left and right sides of the detailed balance expressions (Equations (3) and (9)), termed "detailed imbalance." There is no universal convention for the values of the third component of isospin \( T_3 \) in nucleons, so it is necessary here to indicate the convention in use so as to avoid confusion. This paper considers protons to have \( T_3 = +\frac{1}{2} \), and neutrons to have \( T_3 = -\frac{1}{2} \). This convention was chosen because a proton consists of two up quarks and a down quark (giving it a net "upness"), while a neutron is made from one up quark and two down quarks (yielding a net "downness"). The choice naturally has no effect on the physics, though it does impact nomenclature. To wit, EC and positron emission are isospin-lowering processes, while positron capture and electron emission are isospin-raising processes.

Figure 2 shows the thermal strengths for isospin-lowering CC interactions on \(^{27}\)Al and the reverse reactions on \(^{27}\)Mg, the imbalance in the strengths, and the detailed imbalance at temperatures \( T = 0.17 \) MeV and \( T = 1.0 \) MeV. The tails of the strength distributions fall off rapidly above \(~15\) MeV transition energy (below \(-15\) MeV in the reverse reaction), justifying the truncation in transition energy described above. At both temperatures, the imbalance in thermal strength is overwhelming more than a few MeV from zero transition energy. More importantly, the detailed imbalance is near zero within \(~10\) MeV of the region where the imbalance in thermal strength is not extreme. Therefore, we conclude that detailed imbalance only occurs far out on the tail of one or other of the thermal strength distributions where there is very little strength, which is to say, in regions that do not contribute much to the overall rate of that interaction.

Figure 3 shows the same distributions as Figure 2, but at the extreme temperature of \( T = 3.0 \) MeV. As higher energy nuclear states become populated, the region where the imbalance in thermal strength is small broadens. There remains a gap of a few MeV between this region and the region in which detailed imbalance is large, but the gap is somewhat tenuous, and we might expect some amount of disagreement in the reaction rates as a consequence; I touch on this later.

Figure 4 shows the distributions of forward and reverse NC thermal strength and imbalances for \(^{27}\)Al at temperature \( T = 1.0 \) MeV. We draw the same conclusions as for the CC channel: the detailed imbalance is large only far from where the imbalance in thermal strength is not also extremely large. \(^{27}\)Al is an odd–even nucleus (odd number of protons, even number of neutrons). Because nuclear structure is sensitive to this sort of parity, it is important to ascertain whether these results hold for other kinds of nuclei. Figure 5 shows the CC and NC thermal strength and imbalance for the even–even nucleus \(^{28}\)Si at temperature \( T = 1.0 \) MeV, and Figure 6 shows the same for the odd–odd nucleus \(^{32}\)P. These figures agree with the results for \(^{27}\)Al.

4. Phase-space Factors

Weak reaction rates \( \lambda_i \) between two nuclear states \( |i\rangle \) and \( |j\rangle \) can be expressed as the product of a base rate \( \lambda_0 \) (which contains physical constants), the transition strength \( B_{ij} \) (which is a property of the nucleus), and a phase-space integral \( f_{ij} \) (which accounts for the dynamics of incoming and outgoing particles). Within a given channel, \( \lambda_0 \) and \( B_{ij} \) will be the same for all reactions (though \( B_{ij} \) will of course vary depending on the initial and final states), but the phase-space integral can be qualitatively different for different reactions. For example, in the CC channel, EC from state \( |i\rangle \) to state \( |j\rangle \) and \( \beta^- \) decay from state \( |j\rangle \) to state \( |l\rangle \) have identical relevant physical constants and matrix elements (up to a factor of \((2J_i + 1)/(2J_j + 1)\)), but the phase-space integral of the former must consider electron availability and outgoing neutrino blocking, while the latter must account for outgoing electron and neutrino blocking; Equations (11) and (12) illustrate this.

\[
\Lambda_{ij}^{\text{EC}} = \lambda_0^{\text{EC}} B_{ij}^{-} f_{ij}^{\text{EC}}
\]

\[
f_{ij}^{\text{EC}} = \int_{w_0}^{\infty} dw_e \int_{0}^{\infty} dw_\nu \int_{0}^{\infty} w_e^2 w_\nu^2 G(Z, w_e) \delta(w_e - w_\nu - q_0) \times f_e(1 - f_\nu)
\]

\[
\lambda_{ij}^{\beta^-} = \lambda_0^{\beta^-} B_{ij}^{\beta^-} f_{ij}^{\beta^-} = \lambda_0^{\beta^-} \frac{2J_i + 1}{2J_j + 1} B_{ij}^{-} f_{ij}^{\beta^-}
\]

\[
f_{ij}^{\beta^-} = \int_{w_0}^{q_0} dw_e \int_{0}^{w_e - 1} dw_\nu \int_{0}^{\infty} w_e^2 w_\nu^2 G(Z, w_e) \delta(w_e + w_\nu + q_0) \times (1 - f_e)(1 - f_\nu).
\]
Figure 2. $^{27}$Al isospin-lowering charged-current strength, reverse reaction strength, and imbalance at temperature $T = 0.17$ MeV (left) and $T = 1.0$ MeV (right). The upper panels show the thermal strengths for the forward reactions (solid lines) and reverse reactions ($^{27}$Mg daughter to parent, dashed lines), and the lower panels show the imbalance between the left and right sides of Equation (9) (“detailed imbalance,” solid lines) and in the thermal strength (dashed lines). The large peak in the daughter thermal strengths is from Fermi transitions.

Figure 3. $^{27}$Al isospin-lowering charged-current strength (upper) and imbalance (lower) at temperature $T = 3.0$ MeV. Even at this extreme temperature, detailed imbalance is large only where the imbalance in thermal strength is very large, though the gap between large detailed imbalance and small imbalance in thermal strength has become relatively narrow.

Figure 4. $^{27}$Al neutral-current strength (upper) and imbalance (lower) at temperature $T = 1.0$ MeV. All quantities are defined the same as in Figure 2, though here they are labeled “forward” and “reverse” since the parent and daughter nuclei are identical.
phase-space integrals.
\[
\lambda_{ij}^{de} = \lambda_{0}^{NC} B_{ij}^{GT} f_{ij}^{de}
\]
\[
f_{ij}^{de} = \int_{0}^{\infty} dw_{\nu} \int_{0}^{\infty} dw_{\tau} w_{\nu}^{2} w_{\tau}^{2} \delta(w_{\nu} + w_{\tau} - q) \\
\times (1 - f_{\nu})(1 - f_{\tau})
\]
(13)

\[
\lambda_{ij}^{pa} = \lambda_{0}^{NC} B_{ij}^{GT} f_{ij}^{pa}
\]
\[
f_{ij}^{pa} = \int_{0}^{\infty} dw_{\nu} \int_{0}^{\infty} dw_{\tau} w_{\nu}^{2} w_{\tau}^{2} \delta(w_{\nu} + w_{\tau} - q)f_{\nu} f_{\tau}
\]
(14)

As in Equations (11) and (12), all energies are in units of \(m_e\). Here \(w_{\nu}\) and \(w_{\tau}\) are the neutrino and antineutrino energies, respectively, while \(f_{\nu}\) and \(f_{\tau}\) are the respective distribution functions.

In contrast to the other reactions already discussed, the reverse reaction of neutrino scattering is also neutrino scattering, so the phase-space integral is not qualitatively different:

\[
f_{ij}^{pa} = \int_{0}^{\infty} dw_{\nu} w_{\nu}^{2} (w_{\nu} - q)^{2} f_{\nu}(w_{\nu})(1 - f_{\nu}(w_{\nu} - q))
\]
(15)

Because the phase-space integral for scattering is the same forward and reverse, it is not subject to the arguments below, where we see that qualitative differences in the phase-space factors between forward and reverse reactions have a profound effect on reaction rates when the core is out of weak equilibrium. But because the thermal strength distribution of scattering is the same as that for other NC processes, the general arguments about detailed balance apply.

5. Reaction Rates

With the thermal transition strengths and the phase-space factors in hand, we now examine the effects of detailed imbalance of thermal strength on reaction rate calculations.

Table 1 shows the isospin-raising reaction rates for \(^{32}\)P over a wide range of temperatures and densities; the specific values of temperature and density were selected for easy comparison with Oda et al. (1994). The temperature is listed in units of \(10^9\) K \((T_9)\), and the density is listed as the product of the mass density \(\rho\) in g cm\(^{-3}\) and the electron fraction \((\text{electrons per baryon})\) \(Y_e\). Three values are listed for each entry \((\text{temperature, density, and reaction})\): the upper value is the rate computed from the \(^{32}\)P isospin-raising strength found using the technique described in Section 3, the middle one is computed with the same technique, but using the \(^{32}\)S isospin-lowering strength and applying Equation (8), and the lower value is the imbalance between the two; the second method of computing rates obeys detailed balance between \(^{32}\)P and \(^{32}\)S thermal strengths by construction.

Up to temperature \(T_9 = 10\) \((0.862\text{ MeV})\), both methods agree to high precision. At \(T_9 = 30\) \((2.585\text{ MeV})\), however, the detailed balance method predicts e\(^+\) capture rates that are lower than those predicted by the direct calculation method by a factor of \(\sim 1.74\) at all densities. In fact, this implies that explicitly imposing detailed balance in this case causes some strength to be missed at high temperature. Figure 7 shows the thermal isospin-raising strength and imbalance for \(^{32}\)Pa at \(T_9 = 30\). These curves are qualitatively similar to those in Figure 3, which was also at an extreme temperature.

Figure 8 shows the thermal strength of \(^{32}\)P computed in two ways: using Equation (4) (“Direct”) and using Equation (8) (“Detailed balance”). Equation (8) gave the strength used to compute the lower rates in Table 1. The missing high-temperature strength is clear to see in the broad peak from \(\sim 10\) to 20 MeV transition energy and is reflected in the detailed imbalance shown in Figure 7. Evidently, at extremely high temperatures, the positrons have a long enough high-energy tail that the strength in this energy region contributes significantly,
leading to an underestimate of the rate by the detailed balance method. To further understand this discrepancy, consider that the direct method computes strength from parent states, while the detailed balance method computes strength to daughter states. High-energy parent states are suppressed by the Boltzmann factor, but high-energy daughter states are always accessible as long as the incoming lepton has enough energy. The consequence is that the approximation used to directly compute thermal strengths will be very good to high temperatures, but the relatively sparse sampling of high-energy states can lead to errors when using the detailed balance method. We thus conclude that the method of Section 3 adequately satisfies detailed balance of charged-current reaction strengths for temperatures below 1 MeV, and that even up to very high temperatures, the violation of detailed balance does not lead to extreme disagreement in the computed rates. Furthermore, strictly imposing detailed balance may in fact lead to some missing strength.

### 6. Discussion

The strengths of the computational approach in this work are the use of experimental values where available and an experimentally supported theoretical model to compute unmeasured quantities. When conditions are such that measured reactions dominate the thermal strength and hence reaction rates, this technique will match experiment. Furthermore, the shell model used here has shown itself to be reliable, so we may be confident in the results at higher temperatures and densities where measured transitions may play a relatively smaller role. The weaknesses are the same as those of any shell model calculation, namely, the model space was restricted. In this case, it means that negative parity states were not included. Neither were forbidden transitions included in any of the calculations. However, the purpose of this work is simply to address detailed balance in astrophysical conditions, and to this end, this approach serves as a satisfactory example.

The detailed balance approach used in Section 5 is not a specific broadly used technique. Rather, it is a simple adjustment of the direct approach intended to facilitate comparison of the direct calculation against the general notion of thermal detailed balance. As such, it should not be taken too seriously, particularly in light of the results. What it does illustrate, however, is that strictly imposing thermal detailed balance does not necessarily yield better results in astrophysical environments.

In that vein, we must keep in mind the distinction between detailed balance (which refers to the relationship between forward and reverse transition strengths) and weak equilibrium (which refers to equality between forward and reverse reaction rates). While a realistic model must obey detailed balance of strength, violations thereof may be unimportant if the system under consideration is far from equilibrium, since under such conditions, reactions proceed much faster in one direction than the other.

Consider, for example, Equations (11) and (12). The rate formula for de-excitation into neutrino pairs includes blocking factors for the outgoing neutrino and antineutrino, while the reverse
The Astrophysical Journal, 844:20 (10pp), 2017 July 20

Misch

Table 1
Isospin-raising Reaction Rates for $^{32}$P

| $\rho Y_e$ (g cm$^{-3}$) | Reaction | $T_9 = 0.1$ | $T_9 = 0.7$ | $T_9 = 3.0$ | $T_9 = 10.0$ | $T_9 = 30.0$ |
|-------------------------|----------|-------------|-------------|-------------|-------------|-------------|
| 10                      | $e^-$ capture | $8.7094 \times 10^{-9}$ | $3.9442 \times 10^{-12}$ | $1.5331 \times 10^{-7}$ | $2.0213 \times 10^{-4}$ | $4.7033 \times 10^{-1}$ |
|                         | $e^-$ emission | $1.7740 \times 10^{-8}$ | $1.2179 \times 10^{-8}$ | $1.2251 \times 10^{-6}$ | $1.1197 \times 10^{-4}$ | $7.0098 \times 10^{-3}$ |
| $10^3$                  | $e^+$ capture | $2.6570 \times 10^{-64}$ | $1.4528 \times 10^{-15}$ | $1.3395 \times 10^{-7}$ | $2.0167 \times 10^{-4}$ | $4.7029 \times 10^{-1}$ |
|                         | $e^-$ emission | $1.7405 \times 10^{-8}$ | $1.2031 \times 10^{-8}$ | $1.2237 \times 10^{-6}$ | $1.1195 \times 10^{-4}$ | $7.4477 \times 10^{-3}$ |
| $10^{10}$               | $e^+$ capture | $0.0000$ | $4.0964 \times 10^{-92}$ | $3.5295 \times 10^{-26}$ | $6.6638 \times 10^{-10}$ | $1.3834 \times 10^{-2}$ |
|                         | $e^-$ emission | $0.0000$ | $8.9246 \times 10^{-71}$ | $1.5983 \times 10^{-19}$ | $9.2190 \times 10^{-8}$ | $1.3847 \times 10^{-3}$ |

Note. For each entry ($\rho Y_e$, temperature, and reaction), the upper value is the rate computed using transition strengths found from the technique described in Section 3, the middle value is the rate calculated with that technique, but using the $^{32}$S isospin-lowering strength and applying Equation (8), and the lower value is the imbalance between the rates. The temperature is in units of $10^8$ (K) ($T_9$), and the units of the rates are $s^{-1}$ baryon$^{-1}$.

Figure 7. $^{32}$P isospin-raising charged-current strength (upper) and imbalance (lower) at temperature $T_9 = 30$ (2.585 MeV). As in Figure 3, the region of small strength imbalance is broad.

We conclude that when computing nonequilibrium rates of nuclear weak interactions, particularly in the extreme conditions of stellar and supernova interiors, it is sufficient to directly compute the forward reaction to an appropriate precision without concerning ourselves about whether the particular method strictly obeys detailed balance (though we have already shown that the approach used here largely does).

I gratefully thank George M. Fuller, Yang Sun, and Surja K. Ghorui for fruitful discussions. I also owe gratitude to Projjwal Banerjee, Alice Shih, and Joe Semmelrock for their input in writing this manuscript. This research at Shanghai Jiao Tong University is supported by the National Natural Science Foundation of China (No. 11575112), by the National Key Program for S&T Research and Development (No. 2016YFA0400501), and by the 973 Program of China (No. 2013CB834401).
References

Arnett, W. D. 1977, ApJ, 218, 815
Asakura, K., Gando, A., Gando, Y., et al. 2016, ApJ, 818, 91
Auerbach, N., Bertsch, G., Brown, B., & Zhao, L. 1993, NuPhA, 556, 190
Axel, P. 1962, PhRv, 126, 671
Bazin, D., Montes, F., Becerril, A., et al. 2008, PhRvL, 101, 252501
Bethe, H. A., Brown, G. E., Applegate, J., & Lattimer, J. M. 1979, NuPhA, 324, 487
Brink, D. M. 1955, PhD thesis, Oxford Univ.
Brown, B. A., Chung, W., & Wildenthal, B. H. 1978, PhRvL, 40, 1631
Brown, B. A., Etchegoyen, A., Godwin, N. S., et al. 2004, MSU-NSCL Rep. No. 1289
Brown, B. A., & Richter, W. A. 2006, PhRvC, 74, 034315
Brown, B. A., & Wildenthal, B. H. 1985, ADNDT, 33, 347
Brown, B. A., & Wildenthal, B. H. 1988, ARNPS, 38, 29
Caurier, E., Martínez-Pinedo, G., & Nowacki, F. 1999, NuPhA, 653, 439
Cole, A. L., Anderson, T. S., Zegers, R. G. T., et al. 2012, PhRvC, 86, 015809
Dzhioev, A. A., Vdovin, A. I., Ponomarev, V. Y., et al. 2010, PhRvC, 81, 015804
Dzhioev, A. A., Vdovin, A. I., & Wambach, J. 2015, PhRvC, 92, 045804
Engel, J., Bender, M., Dobaczewski, J., Nazarewicz, W., & Surman, R. 1999, PhRvC, 60, 014302
Fischer, T., Langanke, K., & Martínez-Pinedo, G. 2013, PhRvC, 88, 065804
Fuller, G. M., Fowler, W. A., & Newman, M. J. 1980, ApJS, 42, 447
Fuller, G. M., Fowler, W. A., & Newman, M. J. 1982a, ApJS, 52, 715
Fuller, G. M., Fowler, W. A., & Newman, M. J. 1982b, ApJS, 48, 279
Fuller, G. M., Fowler, W. A., & Newman, M. J. 1985, ApJ, 293, 1
Gao, Z.-C., Sun, Y., & Chen, Y.-S. 2006, PhRvC, 74, 054303
Grover, J. R., & Gilat, J. 1967, PhRv, 157, 802
Hara, K., & Sun, Y. 1995, JIMPE, 4, 637
Hidepolh, L., Müller, B., Janka, H.-T., Marek, A., & Raffelt, G. G. 2010, PhRvL, 104, 251101
Itoh, N., Hayashi, H., Nishikawa, A., & Kohyama, Y. 1996, ApJS, 102, 411
Johnson, C. W., Koonin, S. E., Lang, G. H., & Ormand, W. E. 1992, PhRvL, 69, 3157
Koonin, S. E., Dean, D. J., & Langanke, K. 1997, PhR, 278, 1
Kratz, K.-L. 1988, RevMA, 1, 184
Kratz, K.-L., Gabelmann, H., Hillebrandt, W., et al. 1986, ZPhyA, 325, 489
Langanke, K., & Martínez-Pinedo, G. 2000, NuPhA, 673, 481
Langanke, K., & Martínez-Pinedo, G. 2001, ADNDT, 79, 1
Langanke, K. 2015, in AIP Conf. Proc. 1645, Exotic Nuclei and Nuclear/Particle Astrophysics (V), From Nuclei to Stars, ed. L. Trache et al. (Melville, NY: AIP), 101, doi:10.1063/1.4909564
Lattimer, J. M., Pethick, C., Prakash, M., & Haensel, P. 1991, PhRvL, 66, 2701
Lauritsen, B. 1988, NuPhA, 489, 237
Martínez-Pinedo, G., Lam, Y. H., Langanke, K., Zegers, R. G. T., & Sullivan, C. 2014, PhRvC, 89, 045806
Misch, G. W., & Fuller, G. M. 2016, PhRvC, 94, 055808
Misch, G. W., Fuller, G. M., & Brown, B. A. 2014, PhRvC, 90, 065808
Mori, K., Famiano, M. A., Kajino, T., et al. 2016, ApJ, 833, 179
Nomoto, K. 1987, ApJ, 322, 206
Oda, T., Hino, M., Muto, K., Takahara, M., & Sato, K. 1994, ADNDT, 56, 231
Odrzywolek, A., Misiaszek, M., & Kutschera, M. 2004, APS, 21, 303
Page, D., & Applegate, J. H. 1992, ApJL, 394, L17
Patton, K. M., Lunardini, C., & Farmer, R. J. 2017, ApJ, 840, 2
Richter, W., Mkhize, S., & Brown, B. A. 2008, PhRvC, 78, 064302
Sarriguren, P. 2013, PhRvC, 87, 045801
Sarriguren, P., Alvarez-Rodriguez, R., & De Guerra, E. M. 2005, EPJA, 24, 193
Schweninger, R., Massarczyk, R., Brown, B. A., et al. 2010, PhRvC, 81, 054315
Sun, Y. 2016, PhyS, 91, 043005
Thomas, T. D. 1964, NuPh, 53, 558
Thomas, T. D. 1968, ARNPS, 18, 343
Xu, Z. Y., Nishimura, S., Lorusso, G., et al. 2014, PhRvL, 113, 032505
Zhao, L., & Brown, B. A. 1993, PhRvC, 47, 2641