Approximate Approaches for Nuclear Weak Interaction Rates in Astrophysics

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Nuclear weak interactions, like beta decay, are important inputs for modeling astrophysical explosions. In the allowed approximation, these processes proceed as Fermi or Gamow Teller (GT) processes where the spins of the electron and neutrino are anti-parallel or parallel, respectively. In the GT case, transition probability is spread over many final states in the daughter nucleus, with each probability determination requiring numerical integration of the available phase space. Developing a fast and accurate method for calculating each contribution to the total decay rate would provide reliable weak rate libraries for astrophysical modelers. The phase space integrand includes the classical statistical factor, a Coulomb correction, and the Fermi Dirac distribution of continuum electrons in the stellar material. In this paper, we specifically examine the phase space integration and discuss various approximations to the Coulomb correction, comparing computational speed and numerical accuracy. An approximate approach that is fast and accurate is introduced.

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I. INTRODUCTION

An open question in cosmology is what processes are responsible for the creation of elements heavier than iron. The fusion of lighter elements, such as hydrogen into helium like in the Sun, releases energy up to the silicon-silicon fusion process, but fusion producing elements heavier than iron requires tremendous outside energy input in order to occur. This means explosive astrophysical conditions must somehow be necessary to explain the existence of heavy elements such as gold, thorium or uranium.

Events like supernova explosions and neutron star mergers are leading candidates for the sites of the processes that create heavy elements (see Hitt, 2016 and references therein). Such events have in common a progenitor body made of an exotic state of matter, for example a white dwarf star or a neutron star, where electrons are packed in its plasma at ultra-high densities. This state is called "electron-degenerate"; a state where the same quantum mechanical forces that prevent two electrons from occupying the same orbit in the atom now prevent the body from collapsing under its own gravity. Under these conditions, nuclear beta decays, which create or destroy electrons, can proceed at rates that are many orders of magnitude different than in a terrestrial lab experiment. Therefore, among many other inputs, it is important to determine reliable estimates of nuclear beta decay rates that reflect the changes caused by the stellar environment.

Beta decay is a form of radioactive decay. In this process, an atomic nucleus releases a neutrino and either absorbs or emits an electron or its anti-particle, a positron. Beta decay is caused by the nuclear weak force, a fundamental interaction between sub-atomic particles. In this paper, we will focus on the electron emitting kind of beta decay and refer to it simply as "beta decay" hereafter, but the results below can be extended to the other three versions of the decay. The emitted electron e^- and neutrino ν are produced by the process represented in the following equation

$$ {}^{A}_{Z}X_N \rightarrow {}^{\;\;A}_{Z+1}X' + e^- + \bar{\nu} \qquad (1) $$

where X is the chemical symbol of the initial nucleus and X' that of the final nucleus, each having mass number A and charges Z and Z+1, respectively. The energy released in the process is determined by the mass difference

$$ Q_{\beta^-} = [m_N({}^{A}_{Z}X) - m_N({}^{\;\;A}_{Z+1}X') - m_e]c^2 \qquad (2) $$

Both the electron and the neutrino share this energy, so

$$ Q_{\beta^-} = T_e + E_{\bar{\nu}} \qquad (3) $$

However, as the sharing is not constrained by a conservation law, the kinetic energy of the emitted electron T_e is distributed over a range of possible values between 0 and Q_{β^-}. This fact is critical for determining how the electron-degenerate conditions in the stellar environment will modify the decay rate.

I now review how the rate of the decay λ and the shape of the distribution of T_e are related in the classic Fermi Theory of Beta Decay, following (Krane, 2005). The rate of decay can be calculated using Fermi's golden rule, which assumes the decay process is weak:

$$ \lambda = \frac{2\pi}{\hbar}\left|V_{ji}\right|^2 \rho(E_j) \qquad (4) $$

where V_{ji} is the matrix element that represents the integration of the interaction strength V across the initial i and final j nuclear wavefunctions $\psi_{i,j}$.

$$ V_{ji} = \int \psi_j^* V \psi_i \, dv \qquad (5) $$

Determining V_{ji} is a complicated nuclear structure problem, but is not necessary for our purposes and is beyond the scope of this project. It is sufficient to point out that the number of *j-i* combinations is extremely large for most nuclei (~10^4 to 10^8), each having its own unique $Q = Q_{ij}$, so the determination of $\rho(E_j)$ and of the contribution λ_{ij} to the total rate λ must also be computed equally many times.

In Fermi's golden rule, $\rho(E_j)$ represents the density of the continuum (free) states which must have openings to accept new electrons if the decay process is to proceed. In the lab environment, nearly all continuum states are open and in the stellar environment, these states are rapidly filled and closed with increasing matter density. When filled continuum states prevent the creation of new decay electrons, the phenomenon is called "Pauli blocking".

The number density of continuum electron states can determined by using spherical coordinates to cancel out the volume that the emitted electron is confined to, assuming that the electron is confined to volume V. The resulting relationship is

$$dn_e = \frac{4\pi p^2 \, dp \, V}{h^3} \tag{6}$$

where p is the electron momentum and h is Planck's constant, making the result dimensionless. Likewise, the number density of continuum neutrino states of neutrino momentum q is

$$dn_v = \frac{4\pi q^2 \, dq \, V}{h^3} \tag{7}$$

To determine the momentum and energy distributions, it is necessary to use the partial decay rate form of Fermi's golden rule for emitted electrons and neutrinos with proper momenta

$$d\lambda = \frac{2\pi}{\hbar} g^2 \left|M_{fi}\right|^2 (4\pi)^2 \frac{p^2 \, dp \, q^2}{h^6} \frac{dq}{dE_j} \tag{8}$$

Here, all variables that are not dependent upon momentum can be represented by a constant, C and need not be considered further. We then obtain a distribution that gives the number of electrons present within a range of momentum from p to $p+ dp$:

$$N(p)\, dp = Cp^2 q^2 \, dp \tag{9}$$

Since $Q = T_e + E_\nu$ and $E = p^2/2m$, we can rewrite the above entirely in terms of electron moment p, electron kinetic energy T_e and the energy release Q.

$$N(p) = \frac{C}{c^2} p^2 (Q - T_e)^2 \tag{10}$$

where c is the speed of light. Written entirely in terms of electron kinetic energy T_e

$$N(T_e) = \frac{C}{c^5} (T_e^2 + 2T_e m_e c^2)^{1/2} (Q - T_e)^2 (T_e + m_e c^2) \tag{11}$$

We now have the shape of the distribution we sought, shown in Fig.1.1. Clearly, the function goes to 0 at $T_e = 0$ and at $T_e = Q$ as expected from the equation, and peaks at about $Q/3$. This means the electron kinetic energy is most likely $Q/3$ in a decay, but can be as low as 0 or as high as Q.

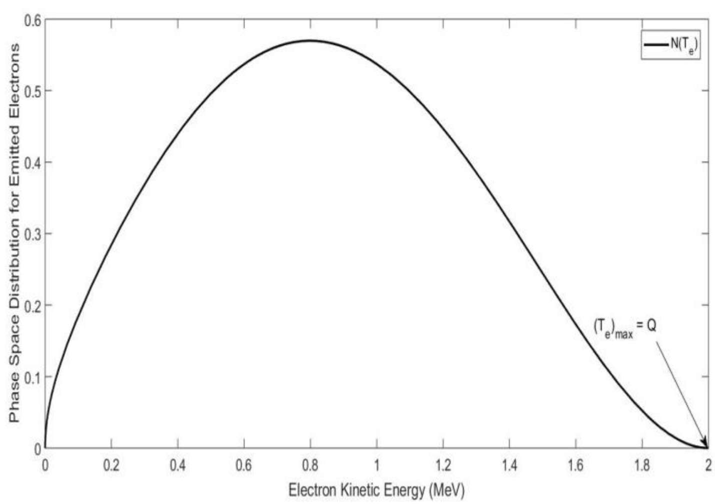

Figure 1.1: The distribution of electron kinetic energy with Q set equal to 2.0 MeV.[1]

To determine the decay rate, ordinarily, one must integrate the distribution in Fig. 1.1, finding the area under the curve, which is the total probability

$$f_{ij} = \int N(T_e, Q_{ij})\, dT_e \tag{12}$$

However, for astrophysics, one must modify the distribution shape to account for electrical interaction with the daughter nucleus (the "Coulomb correction"), modify the distribution shape again, to account for Pauli blocking by electrons already present in the stellar matter, then integrate over T_e, finding the area under the curve in the resulting distribution.

The decay rates in these conditions can be calculated in several ways and, if done quickly, it has potential to save large amounts of CPU time that astrophysicists can then repurpose to other problems in their computer models. For the remainder of the paper, an approximate approach for modifying and integrating the appropriate electron energy distribution, one that is fast and accurate, will be explored. In Section II, I will follow the formalism for the modification process for the electron energy distribution as laid out by Fuller, Fowler, and Newman (FFN) (Fuller, 1980). The calculation involves the integral of the complex gamma function Γ, which is the most expensive calculation in terms of CPU time. An effective term can be found inside the integral, which in Section III, I will show makes a useful approximation that speeds up the calculation while sacrificing little accuracy. In Section IV, I will draw conclusions and outline future work.

II. METHODOLOGY

The total decay rate λ is defined by FFN by double sum over contributions from all *i-j* combinations,

$$\lambda = \sum_{ij} \ln[\frac{2\, f_{ij}(T,\rho,U_F)}{(ft)_{ij}}] \qquad (13)$$

which contains two important terms. The first is the comparative half-life formula ft_{ij}, which involves the nuclear structure input V_{ji} with which we are not concerned. Our concern is the second term, the total probability or "phase space" integral

$$f_{ij} = \int_1^{q_n} w^2 \left(q_{n,ij} - w\right)^2 G(w, \pm Z)(1 - S_\pm)\, d\omega \qquad (14)$$

where FFN has made three important changes relative to the discussion in Section I of this paper. First, there is a change of variables from (T_e, Q_{ij}) to (w, $q_{n,ij}$) where $w = T_e/m_ec^2$ and $q_{n,ij} = Q_{ij}/m_ec^2$, made for convenience. Second, the Coulomb correction $G(w, \pm Z)$ discussed earlier, is here introduced. Third and most importantly, the term $(1 - S_\pm)$ which models the effect of the stellar conditions is introduced. The integrand of f_{ij} in this form represents the density of states available in the continuum of the stellar matter for a new electron from a decay to occupy.

I briefly describe each of the three factors. The classical term in the phase space integral designates the border of the energy forbidden region outside $0 < T_e < Q$ and so enforces energy conservation.

$$P(w, q) = w^2 (q_n - w)^2 \qquad (15)$$

The term containing the Fermi-Dirac distribution, S_- for electron emission,

$$S_- = \left(\exp\left(\frac{U - U_F}{kT}\right) + 1\right)^{-1} \qquad (16)$$

limits the number of continuum states available at energies lower than U_F, the "Fermi energy", where an electron in the stellar matter are already occupying the state and block decays producing new electrons at that energy. The effect on the distribution (dashed black line) can be seen in *Figure 1.2*, where I have set U_F = 1.6 MeV for illustration. Only the area under the resulting green curve can now contribute to the total probability of decay. The width of this "filtered" distribution is controlled by the temperature of the stellar matter and its average energy kT.

The coulomb correction $G(w, \pm Z)$ is given by the equation

$$G(w, \pm Z) \equiv \left({}^{p}/_{w}\right) F(w, \pm Z) \qquad (17)$$

where the relativistic Coulomb barrier term *F(w,±Z)*, contains the complex gamma function as

$$F(w, \pm Z) \approx 2(1+s)(2pR)^{2(s-1)} e^{\pi\eta} \left|\frac{\Gamma(s+iR)}{\Gamma(2s+1)}\right| \tag{18}$$

However, the additional shape change contributed by this modification to the distribution *P(w,q)* is relatively small compared to that of *(1 – S₋)*. Once *G(w,±Z)* is introduced the integrand of f_{ij} mainly increases in amplitude and is only slightly skewed as seen comparing *Figure 1.2* and *Figure 1.3*. The total probability of a decay is now determined by the area under the solid black curve seen in *Figure 1.3*.

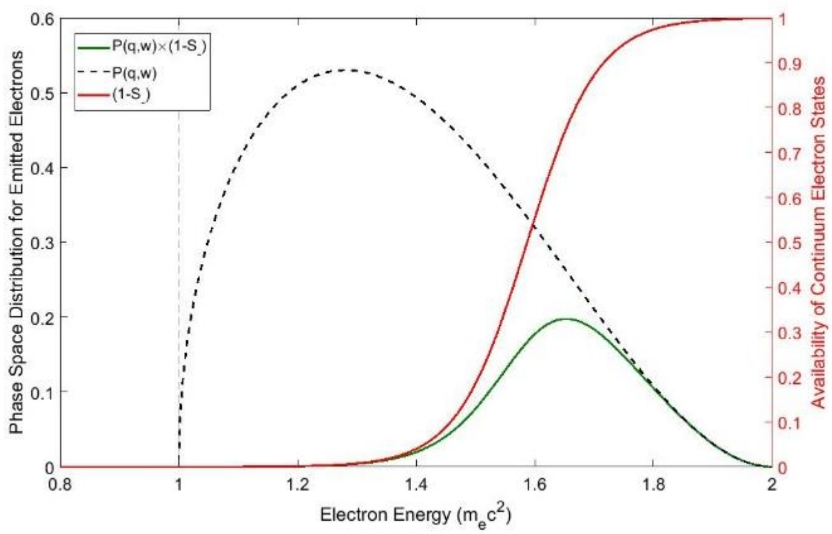

Figure 1.2: The display of the phase space integral without the coulomb correction.

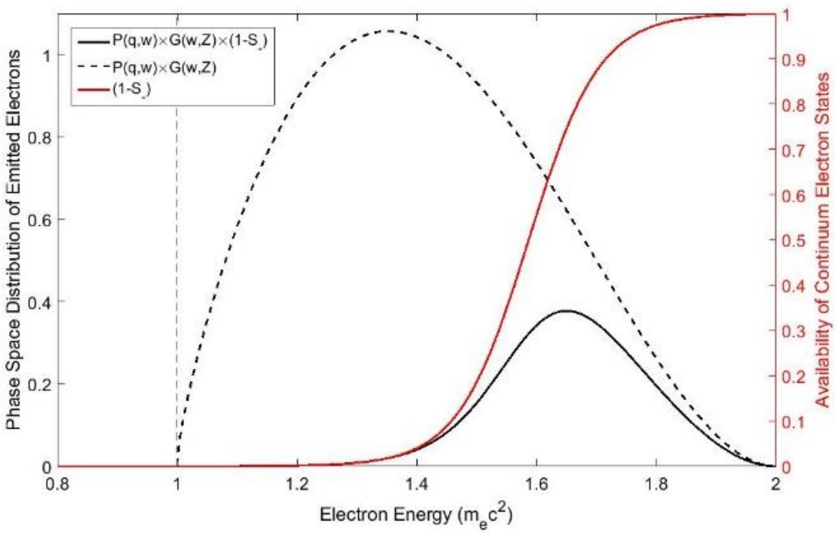

Figure 1.3: Inclusion of the coulomb correction.

To perform the integration faster, a concept for the reverse process of electron capture was suggested by A.D. Becerril-Reyes, S. S. Gupta, et al., where an effective decay rate energy w_{eff} term would be found (Becerril-Reyes, 2006), but this was never put into practice. Because of the now effective decay energy, $G(w,\pm Z)$ becomes $G(w_{eff},\pm Z)$ and is treated as a constant, which can be pulled out of the integrand saving some amount of CPU computing time. *Figures1.2* and *Figure1.3* displays the difference between when the $G(w,\pm Z)$ is and is not included in the integrand. The effective decay energy w_{eff} is determined by finding the average value of the Pauli blocked energy distribution (green curves) in *Figure 1.2* and *Figure 1.4*. The integral of interest, the solid black curve in *Figure 1.3* and *Figure 1.4* is then approximately found by integrating the green curve and multiplying the result by the constant G_{eff}.

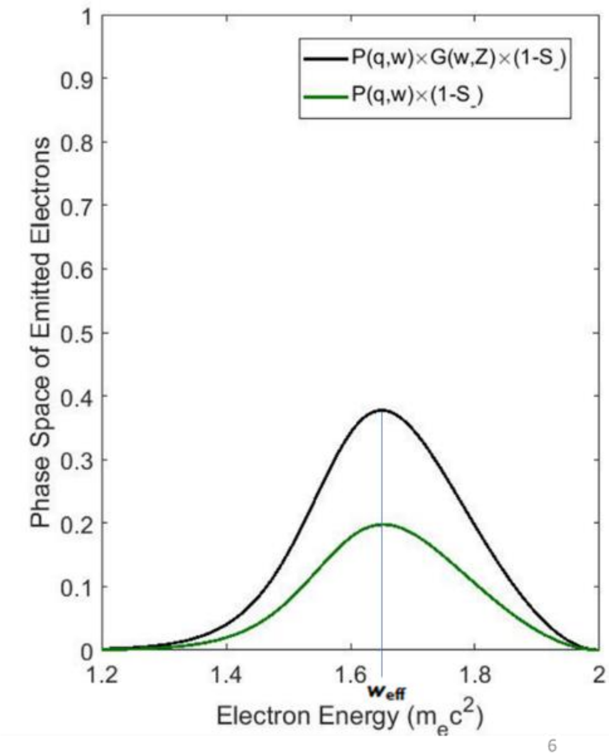

Figure 1.4:Here, the scaling factor is emphasized by w_{eff}.

To find w_{eff}, let the average value of *P(w,q)* be *<P(w,q)>* weighted by the term containing the Fermi-Dirac distribution *(1 – S₋)*

$$< P(w,q) >= \frac{\int_1^{q_n} P(w,q)(1-S_-)\,dw}{\int_1^{q_n}(1-S_-)\,dw} \qquad (19)$$

Let the average value *<P(w,q)>* coincide with the effective decay energy such that

$$< P(w,q) >= w_{eff}^2\left(q_n - w_{eff}\right)^2 \qquad (20)$$

Setting these two equations equal to each other gives a quartic equation in w_{eff}, but one that is already in a reduced form so that it is equivalent to solving a quadratic equation. There are then four roots, but only

$$w_{eff} = \frac{-q-\sqrt{q^2-4\sqrt{<P>}}}{-2} \qquad (21)$$

provides a real (non-imaginary) value that doesn't fall in the energy forbidden region outside $1 < w < q$.

III. RESULTS

A histogram in *Figure 4* was created to display the speed up factor and accuracy of performing the integration with the effective Coulomb correction G_{eff} over that of leaving the full functional form $G(w,\pm Z)$ in the integrand (Anderson, 2017). The calculations for the plot were done over a total of 12,000 cases, spread over a grid with ranges listed as follows: total decay energy q from 2 to 50 (larger than any real beat decay), the nuclear charge Z from 10 to 120 in steps of 10, the Fermi energy of continuum electrons in the stellar material U_F from 1 to 200 MeV (corresponding to white dwarf star up to neutron star matter densities, respectively), and the temperature T from 0.01 to 10 billion Kelvins. The corners of the 2D distribution in Figure 1.5 reveal the worst-case and best-case performance for the approximation. The top right corner shows the best-case, where the approximate and exact integrations are essentially equal, but the approximation is 20x faster. The lower left corner shows the worst-case, where the approximate approach underestimates the exact integral by about 50% and is only 18x times faster.

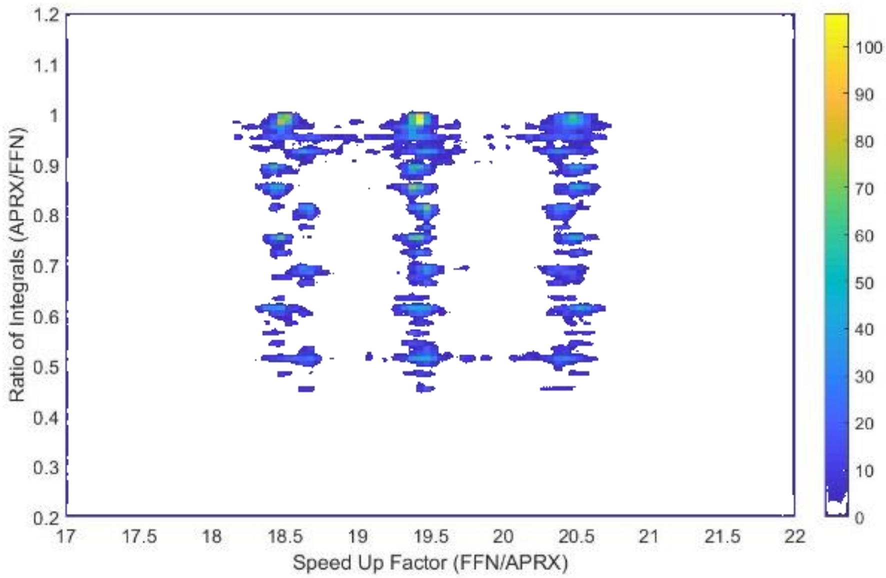

Figure 1.5: The distribution shown by cases per pixel over 12000 cases, spread over astrophysically relevant ranges of temperature, density, nuclear charge and total decay energy.

IV. CONCLUSIONS

In conclusion, the approximate approach for phase space integrations for beta-decay rates under electron-degenerate astrophysical conditions was defined and examined in detail. The approach assigns an effective decay energy w_{eff} and an associated effective Coulomb correction G_{eff}. The results showed that the worst-case scenario is that it has at most 50% error, but is still 18x faster. The best-case scenario is close to a one to one ratio and around 20x faster. Absolute values of beta decay rates in the stellar environment can range over intervals that are dozens, even hundreds of orders-of-magnitude wide, so a worst case error of 50% is certainly an acceptable sacrifice in exchange for performing the calculation 18-20x times faster. Since the effective procedure is quick and accurate to calculate the emission rate for electrons, it could also be useful to develop the same approach conceptually to calculate rates for positron and neutrino emissions and captures. Future work would involve solving the calculations for the weak rates of these related processes.

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