# **Nuclear de-excitations in low-energy charged-current** *ν<sup>e</sup>* **scattering on 40Ar**

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(Received 8 February 2021; accepted 22 February 2021; published 5 April 2021)

**Background:** Large argon-based neutrino detectors, such as those planned for the Deep Underground Neutrino Experiment, have the potential to provide unique sensitivity to low-energy (few to tens of MeV) electron neutrinos produced by core-collapse supernovae. Despite their importance for neutrino energy reconstruction, nuclear de-excitations following charged-current ν*<sup>e</sup>* absorption on 40Ar have never been studied in detail at supernova energies.

**Purpose:** I develop a model of nuclear de-excitations that occur following the <sup>40</sup>Ar(*v<sub>e</sub>*, *e*−)<sup>40</sup>K<sup>∗</sup> reaction. This model is applied to the calculation of exclusive cross sections.

**Methods:** A simple expression for the inclusive differential cross section is derived under the allowed approximation. Nuclear de-excitations are described using a combination of measured  $\gamma$ -ray decay schemes and the Hauser-Feshbach statistical model. All calculations are carried out using a novel Monte Carlo event generator called MARLEY (Model of Argon Reaction Low Energy Yields).

**Results:** Various total and differential cross sections are presented. Two de-excitation modes, one involving only  $\gamma$  rays and the other including single neutron emission, are found to be dominant at few tens-of-MeV energies. **Conclusions:** Nuclear de-excitations have a strong impact on the achievable energy resolution for supernova  $v_e$  detection in liquid argon. Tagging events involving neutron emission, though difficult, could substantially improve energy reconstruction. Given a suitable calculation of the inclusive cross section, the MARLEY nuclear de-excitation model may readily be applied to other scattering processes.

DOI: [10.1103/PhysRevC.103.044604](https://doi.org/10.1103/PhysRevC.103.044604)

# **I. INTRODUCTION**

Core-collapse supernovae are exceptionally intense sources of tens-of-MeV neutrinos and antineutrinos of all flavors. In a typical supernova, about  $10^{58}$  neutrinos are released in a burst lasting tens of seconds. Although the first observation of supernova neutrinos by the Kamiokande-II [\[1\]](#page-18-0), Baksan [\[2\]](#page-18-0), and Irvine-Michigan-Brookhaven [\[3\]](#page-18-0) detectors in 1987 yielded a total of only two dozen events, the scientific impact of this dataset has been tremendous, leading to numerous publications on a wide variety of subjects [\[4–9\]](#page-18-0). In the years since first detection, a worldwide network of large neutrino experiments, most built primarily for other applications, stands ready to perform a second, high-statistics measurement if a core-collapse supernova should occur within the galaxy  $[10]$ . Due to the slow rate of galactic core-collapse supernovae (estimated to be about 1.6 per century [\[11\]](#page-18-0)), the prospect of such a measurement represents a rare but valuable opportunity to shed light on the details

of core-collapse and nucleosynthesis, study neutrinos under extreme conditions, search for evidence of physics beyond the Standard Model, and explore many other topics [\[12–](#page-18-0)[14\]](#page-19-0).

A full realization of the physics potential of the next galactic core-collapse supernova will require a simultaneous measurement of neutrinos of all flavors. While detectors based on water and hydrocarbon scintillator will primarily detect  $\bar{ν}_e$ via inverse  $\beta$  decay (IBD)

$$
\bar{\nu}_e + p \to e^+ + n \,, \tag{1}
$$

liquid-argon-based detectors are anticipated to provide unique sensitivity  $[15,16]$  to  $\nu_e$  via the charged-current (CC) reaction,

$$
\nu_e + {}^{40}\text{Ar} \to e^- + {}^{40}\text{K}^*,\tag{2}
$$

which dominates the expected signal at supernova energies.

Within the decade, the Deep Underground Neutrino Experiment (DUNE) will begin operating four 10-kiloton liquid argon time projection chambers (LArTPCs) with the primary goals of studying long-baseline oscillations of accelerator neutrinos, searching for proton decay, and measuring the ν*<sup>e</sup>* flux from a galactic core-collapse supernova if one should occur during the lifetime of the experiment [\[17\]](#page-19-0). Initial studies of the sensitivity of DUNE to supernova neutrinos, performed by the collaboration itself [\[15\]](#page-19-0) and by smaller groups (e.g., Ref. [\[18\]](#page-19-0)) show promise, and the potential exists for measurements by DUNE of other low-energy neutrinos, notably those produced by the Sun [\[19\]](#page-19-0).

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In addition to DUNE, three subkiloton LArTPCs, SBND [\[20,21\]](#page-19-0), MicroBooNE [\[22\]](#page-19-0), and ICARUS [\[23\]](#page-19-0), are currently operating or being installed in the Booster Neutrino Beam at Fermilab. A joint effort between the three experimental collaborations, known as the Short Baseline Neutrino (SBN) program [\[24,25\]](#page-19-0), will perform precision measurements of neutrino oscillations. In addition to this primary mission, the SBN detectors will pursue a variety of other physics measurements and are expected to be sensitive to supernova neutrinos. To ensure that data from a core-collapse supernova would be fully recorded over the ten-second burst, the MicroBooNE collaboration operates a first-of-its-kind continuous readout stream and has demonstrated its capabilities via reconstruction of Michel electrons produced by decays of cosmic muons [\[26\]](#page-19-0).

While much remains to be done to fully exploit the lowenergy capabilities of LArTPCs, a first demonstration by the ArgoNeuT [\[27\]](#page-19-0) experiment of reconstruction of MeVscale activity due to accelerator-neutrino-induced neutrons and de-excitation  $\gamma$  rays achieved a detection threshold of around 200–300 keV [\[28\]](#page-19-0). These encouraging initial results have prompted further experimental work by MicroBooNE [\[29\]](#page-19-0) and multiple simulation-based studies considering the implications for reconstruction of both high- and low-energy physics events [\[30,31\]](#page-19-0).

In future analyses of supernova neutrino data, the event-byevent reconstructed neutrino energy obtained by each detector will be of primary interest. For IBD events in water or scintillator, because only a single hadronic final state (a free neutron) is accessible at tens-of-MeV energies, a measurement of the outgoing positron energy is sufficient to reconstruct the antineutrino energy with high accuracy. Due to the use of a complex nuclear target (argon) in LArTPCs, however, various nuclear transitions may occur in response to CC ν*<sup>e</sup>* absorption, and thus a one-to-one mapping (up to nuclear recoil) between the neutrino and electron energies no longer exists.

To fully reconstruct the neutrino energy in the argon case, the reaction *Q* value, i.e., the energy imparted to the nuclear transition, must be inferred by detecting the nuclear deexcitation products. For transitions to bound nuclear energy levels, the neutrino energy is in principle fully recoverable by measuring the energies of all de-excitation  $\gamma$  rays in addition to the primary electron. For transitions to unbound nuclear states, a model is needed to correct for missing energy associated with undetected nuclear fragments. In practice, an experimental analysis that attempts to isolate the simpler bound transitions will also need a detailed de-excitation model in order to estimate the purity of the event selection.

With the exception of a recent first measurement [\[32\]](#page-19-0) of coherent elastic neutrino-nucleus scattering, experimental data have not yet been obtained for neutrino-argon cross sections in the supernova energy regime. Furthermore, only a few measurements with limited precision are available for low-energy inelastic neutrino scattering on any nuclear target [[\[33\]](#page-19-0), table 3]. Despite this, a substantial literature exists for theoretical calculations of the <sup>40</sup>Ar( $v_e$ ,  $e^{-}$ )<sup>40</sup>K<sup>\*</sup> process. A review through 2018 is provided in Ref. [[\[34\]](#page-19-0), Sec. 7.1], with a notable recent addition being two publications [\[35,36\]](#page-19-0) which employ a continuum random-phase approximation (CRPA) model to study this cross section above the nucleon emission threshold.

While highly useful for providing competing estimates of event rates in DUNE and other argon-based detectors, all published calculations for this cross section to date share the limitation of being fully inclusive, i.e., predictions are made that consider only the kinematics of the outgoing electron. At very low neutrino energies, where only transitions to bound nuclear states are possible, this is not problematic: Measured de-excitation  $\gamma$ -ray branching ratios exist for many levels of the daughter  ${}^{40}K$  nucleus, and missing data may be addressed using straightforward theoretical estimates. However, above about 15–20 MeV, kinematic access to unbound nuclear states becomes appreciable, and a detailed treatment of the competition between various de-excitation channels (including emission of both  $\gamma$  rays and nuclear fragments) is needed.

Although such a treatment has not previously been provided for  $40$ Ar, detailed modeling of nuclear de-excitations induced by low-energy neutrino interactions has been pursued for a number of other nuclei [\[37–42\]](#page-19-0). A universal assumption made by all of these calculations (as well as the present work) is that of *compound nucleus* formation: Following the primary interaction, the nucleus is left in a thermally equilibrated excited state that decays independently of the details of its formation process. While further work is needed to fully investigate the adequacy of this assumption for low-energy neutrino-nucleus reactions, both theoretical calculations  $[43,44]$  and electron scattering data  $[45]$  suggest that compound processes dominate over the direct nucleon knock-out important at higher energies.

In this paper, I present the first calculations at tens-of-MeV energies for cross sections for exclusive final states of the reaction <sup>40</sup>Ar( $v_e$ ,  $e^{-}$ )<sup>40</sup>K<sup>\*</sup>, emphasizing the role of nuclear de-excitation processes. In Sec. [II,](#page-2-0) I develop a simple model for the inclusive differential cross section, relying on approximations that work best at low momentum transfers. The derivation in Sec.  $\Pi$  fully determines the cross section up to the values of two (Fermi and Gamow-Teller) nuclear matrix elements, *B*(F) and *B*(GT), which are considered in Sec. [III.](#page-4-0) While relevant neutrino scattering data are currently unavailable, the needed values of these matrix elements at low excitation energies may be extracted from measurements of related processes. I supplement these measurements with the results of a theoretical calculation at high excitation energies to obtain a full treatment of the inclusive cross section. In Sec. [IV,](#page-6-0) I describe a detailed model of nuclear de-excitations that can be used together with the inclusive cross section to obtain predictions for exclusive final states. In Sec. [V,](#page-9-0) I present example results calculated using the models developed in the previous sections.

To enable practical calculations that have already helped to inform studies of DUNE's sensitivity to supernova neutrinos [\[15\]](#page-19-0), all of the physics models described herein have been implemented in a new Monte Carlo event generator called MARLEY (Model of Argon Reaction Low Energy Yields). All results shown in this work may be reproduced using version 1.2.0 of MARLEY [\[46\]](#page-20-0), which is publicly available as an opensource software project [\[47\]](#page-20-0). Documentation of the technical <span id="page-2-0"></span>details of MARLEY and usage instructions are available in Ref. [\[48\]](#page-20-0).

Due to the compound nucleus assumption, the MARLEY deexcitation model may easily be used in the future to provide exclusive predictions for a more refined calculation of the inclusive CC  $v_e$  absorption cross section for <sup>40</sup>Ar. A similar approach to modeling de-excitations for other reaction modes and target nuclei is likewise possible, and I welcome potential collaboration on this topic. Prospects for improving MARLEY predictions beyond the proof-of-concept reported here are briefly considered in Sec. [VI.](#page-15-0)

#### **II. INCLUSIVE CROSS-SECTION MODEL**

For momentum transfers that are small compared to the *W* boson mass, the tree-level amplitude  $M$  for inclusive charged-current neutrino-nucleus scattering may be represented diagramatically as



The corresponding differential cross section may be written in the form

$$
\frac{d\sigma}{dQ^2} = \frac{G_F^2 |V_{ud}|^2}{32 \pi (s - m_i^2)^2} F_C L_{\mu\nu} W^{\mu\nu},\tag{4}
$$

where  $q = k - k' = p' - p$  is the four-momentum transfer,  $Q^2 \equiv -q^2$ ,  $G_F$  is the Fermi constant,  $V_{ud}$  is the Cabibbo-Kobayashi-Maskawa matrix element connecting the up and down quarks, Mandelstam *s* is the square of the total energy in the center-of-momentum  $(CM)$  frame, and  $m_i$  is the mass of the initial-state nucleus. Discussion of the Coulomb correction factor  $F_C$  is deferred to Sec. [II B.](#page-3-0)

The leptonic ( $L_{\mu\nu}$ ) and hadronic ( $W^{\mu\nu}$ ) tensors are defined by

$$
L_{\mu\nu} \equiv \text{Tr}[\gamma_{\mu} (1 - \gamma_5) \, k \, \gamma_{\nu} (1 - \gamma_5) \, (\not{k}' + m_{\ell})], \tag{5}
$$

$$
= 8[k_{\mu} k'_{\nu} + k_{\nu} k'_{\mu} - g_{\mu\nu} (k \cdot k') - i\epsilon_{\mu\nu\rho\sigma} k^{\rho} k'^{\sigma}], \tag{6}
$$

and

$$
\mathsf{W}^{\mu\nu} \equiv \frac{1}{2J_i + 1} \sum_{M_i} \sum_{M_f} \mathcal{N}^{\mu} \, \mathcal{N}^{\nu*}.\tag{7}
$$

Here  $m_\ell$  is the mass of the final-state lepton,  $J_i$  ( $J_f$ ) is the initial (final) nuclear spin, and  $M_i$  ( $M_f$ ) is the third component of the nuclear spin in the initial (final) state.

Under the impulse approximation, the nuclear matrix element may be written in coordinate space as

$$
\mathcal{N}^{\mu} = \langle f | \sum_{n=1}^{A} e^{i\mathbf{q} \cdot \mathbf{x}(n)} j^{\mu}(n) | i \rangle, \tag{8}
$$

where **q** is the three-momentum transfer and the sum runs over all *A* nucleons. The weak current operator  $j^{\mu}(n)$  is understood to act only on the *n*th nucleon, as is the position operator  $\mathbf{x}(n)$ . The state vectors in Eq. (8) are normalized relativistically, i.e.,

$$
\langle i|i\rangle = 2E_i, \quad \langle f|f\rangle = 2E_f, \tag{9}
$$

where  $E_i(E_f)$  is the total energy of the nucleus in the initial (final) state. Equation (4) contains an implied sum over the accessible final nuclear states.

# **A. Allowed approximation**

The full expression for the single-nucleon weak current operator  $j^{\mu}$  is well known and is given in Ref. [\[34\]](#page-19-0) among other places. For this study, however, I evaluate the current operator in the *allowed approximation*, which combines the long-wavelength  $(q \to 0)$  limit and the slow-nucleon limit (in which the momentum of the initial struck nucleon is neglected compared to its mass).

Under this approximation, the weak current operator reduces to the simple form

$$
j^0 = g_V t_- \quad j^a = -\sigma^a \, g_A \, t_-, \tag{10}
$$

where  $j^0$  is the time component and the three Cartesian spatial components are labeled with  $a \in \{1, 2, 3\}$ . The time component of the nuclear matrix element  $\mathcal{N}^{\mu}$  is given by

$$
\mathcal{N}^0 = \frac{g_V}{\sqrt{2J_i+1}} \,\delta_{J_i J_f} \,\delta_{M_i M_f} \,\langle f \, \|\mathcal{O}_F \, \| i \rangle, \tag{11}
$$

while the spatial components may be written in spherical coordinates as

$$
\mathcal{N}^{w} = \frac{-g_{A}(-1)^{J_{i}-M_{i}}}{\sqrt{3}} (J_{f} M_{f} J_{i} - M_{i} | 1 w) \langle f \| \mathcal{O}_{GT} \| i \rangle,
$$
\n(12)

where  $w \in \{-1, 0, 1\}$  and  $g_V(g_A)$  is the vector (axial-vector) weak coupling constant of the nucleon. The Fermi (F) and Gamow-Teller (GT) operators are defined by

$$
\mathcal{O}_F \equiv \sum_{n=1}^A t_-(n),\tag{13}
$$

$$
\mathcal{O}_{GT} \equiv \sum_{n=1}^{A} \sigma(n) t_{-}(n), \qquad (14)
$$

where *σ* is the Pauli vector, and *t*−, the isospin-lowering operator, converts a neutron into a proton. Double bars (||) denote matrix elements which have been reduced via the Wigner-Eckhart theorem.

Equations  $(11)$  and  $(12)$  may be used to evaluate the elements of the hadronic tensor  $W^{\mu\nu}$ . Under the allowed <span id="page-3-0"></span>approximation, these become

$$
\mathsf{W}^{00} = 4 E_i E_f B(\mathsf{F}) \tag{15}
$$

$$
\mathsf{W}^{ab} = \frac{4}{3} \, \delta_{ab} \, E_i \, E_f \, B(\text{GT}) \tag{16}
$$

$$
\mathsf{W}^{0a} = \mathsf{W}^{a0} = 0,\tag{17}
$$

where the reduced Fermi and Gamow-Teller matrix elements are given by

$$
B(\mathbf{F}) \equiv \frac{g_V^2}{2J_i + 1} |\langle J_f \parallel \mathcal{O}_F \parallel J_i \rangle|^2, \tag{18}
$$

$$
B(\text{GT}) \equiv \frac{g_A^2}{2J_i + 1} |\langle J_f \parallel \mathcal{O}_{\text{GT}} \parallel J_i \rangle|^2. \tag{19}
$$

The state vectors labeled using the nuclear spin  $(J_i \text{ or } J_f)$  are normalized to unity:

$$
\langle J_i | J_i \rangle = \langle J_f | J_f \rangle = 1. \tag{20}
$$

The reduced matrix elements satisfy the spin-parity selection rules

$$
B(F) = 0 \text{ unless } J_f = J_i \text{ and } \Pi_f = \Pi_i \tag{21}
$$

and

$$
B(\text{GT}) = 0 \text{ unless } |J_i - 1| \leqslant J_f \leqslant J_i + 1 \text{ and } \Pi_f = \Pi_i. \tag{22}
$$

where  $\Pi_i$  ( $\Pi_f$ ) is the initial (final) nuclear parity.

Combining the results above leads to the following expression for the allowed approximation differential cross section in the CM frame:

$$
\frac{d\sigma}{d\cos\theta_{\ell}} = \frac{G_F^2 |V_{ud}|^2}{2\pi} F_C \left[\frac{E_i E_f}{s}\right] E_{\ell} |\mathbf{p}_{\ell}| \left[ (1 + \beta_{\ell} \cos \theta_{\ell}) B(\mathbf{F}) + \left(1 - \frac{1}{3} \beta_{\ell} \cos \theta_{\ell}\right) B(\mathbf{GT}) \right].
$$
\n(23)

Here  $E_{\ell}$ ,  $\mathbf{p}_{\ell}$ ,  $\theta_{\ell}$ , and  $\beta_{\ell} = E_{\ell}/|\mathbf{p}_{\ell}|$  are, respectively, the total energy, three-momentum, scattering angle, and speed of the final-state lepton. The factor  $E_i E_f / s$  accounts for nuclear recoil and is commonly neglected.

In the CM frame, the particle energies are independent of the scattering angle  $\theta_{\ell}$ . As a result, integration of the total cross section is trivial and leads to the expression

$$
\sigma = \frac{G_F^2 |V_{ud}|^2}{\pi} F_C \left[ \frac{E_i E_f}{s} \right] E_\ell |\mathbf{p}_\ell| [B(\mathbf{F}) + B(\mathbf{GT})]. \tag{24}
$$

As was the case for Eq. [\(4\)](#page-2-0), the cross-section formulas in Eqs. (23) and (24) contain an implicit sum over nuclear final states.

#### **B. Coulomb corrections**

Final-state interactions (FSIs) of the outgoing charged lepton with the Coulomb field of the nucleus have a significant effect on the cross section at low energies. While a detailed treatment of Coulomb FSIs is achievable via the distorted-wave Born approximation, a much more convenient approximation scheme based on the work of Engel [\[49\]](#page-20-0) is typically used, e.g., in Refs. [\[35,](#page-19-0)[50,51\]](#page-20-0).

Under this approach, the Coulomb correction factor  $F_C$ that appears in Eqs.  $(4)$ ,  $(23)$ , and  $(24)$  is calculated using either the Fermi function [\[52,53\]](#page-20-0) or the modified effective momentum approximation (MEMA) [\[49\]](#page-20-0). Since the former is known to overestimate Coulomb corrections at high lepton energies while the latter does the same at low energies, the smaller of the two alternatives is always chosen. This amounts to defining the Coulomb correction factor as

$$
F_C \equiv \begin{cases} F_{\text{Fermi}} & |F_{\text{Fermi}} - 1| < |F_{\text{MEMA}} - 1| \\ F_{\text{MEMA}} & \text{otherwise} \end{cases} \tag{25}
$$

where the Fermi function is given by

$$
F_{\text{Fermi}} = \frac{2(1+S)}{[\Gamma(1+2S)]^2} (2 \gamma_{\text{rel}} \beta_{\text{rel}} m_{\ell} R)^{2S-2}
$$
  
×  $e^{-\pi \eta} |\Gamma(S - i\eta)|^2$  (26)

and

$$
F_{\text{MEMA}} \equiv \frac{\mathcal{K}_{\text{eff}} \,\mathcal{E}_{\text{eff}}}{\mathcal{K}\mathcal{E}}.\tag{27}
$$

In Eq.  $(26)$  the quantity *S* is defined in terms of the fine structure constant  $\alpha$  by

$$
S \equiv \sqrt{1 - \alpha^2 Z_f^2},\tag{28}
$$

where  $Z_f$  is the proton number of the final nucleus. The nuclear radius (in natural units) may be estimated as

$$
R \approx \frac{1.2 A^{1/3} \text{ fm}}{\hbar c},\qquad(29)
$$

and the Sommerfeld parameter  $\eta$  is given by

$$
\eta = \frac{\alpha Z_f z_\ell}{\beta_{\text{rel}}},\tag{30}
$$

where  $z_{\ell}$  is the electric charge (in units of the elementary charge) of the final-state lepton.

Typical presentations of the correction factors defined in Eqs. (26) and (27) neglect the small recoil kinetic energy of the final nucleus in the laboratory frame. This allows the use of expressions for  $F_{\text{Fermi}}$  and  $F_{\text{MEMA}}$  which are derived in the rest frame of the final nucleus. I opt instead for Lorentz-invariant forms of the correction factors written in terms of the relative speed  $\beta_{rel}$  of the two final-state particles [\[54\]](#page-20-0):

$$
\beta_{\text{rel}} = \frac{\sqrt{(k' \cdot p')^2 - m_{\ell}^2 m_f^2}}{k' \cdot p'} \quad \gamma_{\text{rel}} \equiv \left(1 - \beta_{\text{rel}}^2\right)^{-1/2}.
$$
 (31)

The symbols *E* and *K* from Eq. (27) denote, respectively, the total energy and momentum of the outgoing lepton in the rest frame of recoiling nucleus:

$$
\mathcal{E} \equiv \gamma_{\text{rel}} \, m_{\ell} \quad \mathcal{K} \equiv \beta_{\text{rel}} \, \mathcal{E}. \tag{32}
$$

The *effective* values of these variables are those that exist in the presence of the nuclear Coulomb potential

$$
\mathcal{K}_{\text{eff}} \equiv \sqrt{\mathcal{E}_{\text{eff}}^2 - m_\ell^2} \quad \mathcal{E}_{\text{eff}} \equiv \mathcal{E} - V_C(0),\tag{33}
$$

<span id="page-4-0"></span>which is approximated by that at the center of a uniformly charged sphere:

$$
V_C(0) \approx \frac{3 Z_f z_\ell \alpha}{2R} \,. \tag{34}
$$

It should be noted that, as originally presented [\[49\]](#page-20-0), the MEMA also involves modifying the value of the momentum transfer used to evaluate the amplitude  $M$ . Since the cross-section treatment presented here involves use of the long-wavelength limit  $q \rightarrow 0$ , however, I neglect this additional correction.

# **III. ALLOWED NUCLEAR MATRIX ELEMENTS**

Despite sustained community interest and a concrete proposal by the CAPTAIN experiment [\[55\]](#page-20-0) to perform direct measurements, no experimental data for tens-of-MeV charged-current ν*<sup>e</sup>* scattering on argon are currently available. However, in recent decades, three separate experiments have obtained values of the allowed matrix elements *B*(F) and *B*(GT) by considering related physics processes.

The first two experiments were performed in the late 1990s by separate teams working at the Gesellschaft für Schwerionenforschung (Society for Heavy Ion Research) in Darmstadt, Germany [\[56\]](#page-20-0) and the Grand Accélérateur National d'Ions Lourds (Large Heavy Ion National Accelerator) in Caen, France [\[57\]](#page-20-0). Both sought to study CC  $v_e$  absorption on <sup>40</sup>Ar by measuring  $\beta$  decays of its mirror nucleus <sup>40</sup>Ti:

$$
^{40}\text{Ti} \to {}^{40}\text{Sc}^* + e^+ + \nu_e \,. \tag{35}
$$

In the limit of perfect isospin symmetry, the matrix element describing a <sup>40</sup>Ti  $\beta$  decay transition to a specific <sup>40</sup>Sc level is equal to the matrix element accessing the level's isobaric analog in <sup>40</sup>K via CC  $v_e$  scattering on <sup>40</sup>Ar. The main difficulties in applying this technique to neutrino cross sections are (1) the  $\beta$  decay  $Q$  value limits the maximum excitation energy that may be studied, and (2) energy levels in the  $\beta$  decay daughter nucleus  $(^{40}Sc)$  must be matched to their analogs in the final-state nucleus for neutrino scattering  $(^{40}K)$ .

The third experiment [\[58\]](#page-20-0), performed about a decade later at the Indiana University Cyclotron Facility, extracted *B*(GT) values from measurements of  $(p, n)$  scattering on <sup>40</sup>Ar. The extraction technique relied on the observation, first put for-ward in 1980 [\[59\]](#page-20-0) and subsequently refined [\[60–62\]](#page-20-0), that the  $(p, n)$  cross section at very forward angles  $(\theta \approx 0^{\circ})$  for proton energies around 100 MeV is approximately proportional to the allowed matrix elements  $B(F)$  and  $B(GT)$ . While subject to some unique difficulties of its own (see, e.g., Ref. [[\[63\]](#page-20-0), Sec. 4.2]), this approach overcomes key limitations of  $40$ Ti  $β$  decay: Transitions to excited levels of <sup>40</sup>K may be studied directly at energies higher than the mirror  $\beta$  decay  $Q$  value.

#### **A. Re-evaluation of existing measurements**

Reasonable attempts were made in the original publications describing these measurements to assign the extracted matrix elements to known  ${}^{40}$ K levels satisfying the spin-parity selection rules in Eqs. [\(21\)](#page-3-0)–[\(22\)](#page-3-0). That is, the  ${}^{40}$ K isobaric analog state accessed via a Fermi transition must have  $J^{\pi} = 0^{+}$ , while GT transitions may only populate levels with  $J^{\pi} = 1^{+}$ .

However, in light of new  ${}^{40}$ K level data that became available in 2017 [\[64\]](#page-20-0), I revisited the level assignments for all three measurements.

The results of this re-evaluation are shown in Table [I.](#page-5-0) Level energies (keV) and spin-parity assignments retrieved from the Evaluated Nuclear Structure Data File (ENSDF) database [\[65\]](#page-20-0) are listed in the first and second columns, respectively. Excitation energies (for either  ${}^{40}$ Sc or  ${}^{40}$ K as appropriate) and matrix element values are listed in the following columns for each of the three experimental measurements. In the case of the  $(p, n)$  scattering data, the matrix element values provided in the original paper [\[58\]](#page-20-0) have been scaled by a factor of  $g_A^2 =$ 1.26<sup>2</sup>. This scaling was done because the definition of  $B(GT)$ used by the experiment does not include the axial-vector weak coupling constant  $g_A$ . The specific value  $g_A = 1.26$  was chosen for consistency with the one assumed in the experimental analysis.

Figure [1](#page-6-0) shows the Gamow-Teller strengths obtained by the two  $^{40}$ Ti  $\beta$  decay experiments mentioned previously. Excitation energies of analog states in  ${}^{40}$ K, represented on the horizontal axis, are chosen to match the assignments made in Table [I.](#page-5-0) The vertical axis is inverted for the second dataset to facilitate comparisons. Rough consistency is seen between the two measurements, although the results reported by Liu *et al.* involve several more nuclear levels.

Figure [2](#page-6-0) uses a similar format to individually compare each  $\beta$  decay measurement to the GT strengths extracted from (*p*, *n*) scattering. Substantially more fragmentation of the strength is seen in the  $\beta$  decay data, and there are areas of significant tension. For instance, the two experimental methods disagree on whether the GT strength to the  $^{40}$ K level at 2.3 MeV is larger or smaller than the strength to the level at 2.7 MeV.

Differences between the  $\beta$  decay and  $(p, n)$  data were examined in detail by Karakoç *et al.* in 2014 [\[67\]](#page-20-0). Based on a combination of theoretical calculations and a currently unpublished  $^{40}Ar(h, t)$   $^{40}K$  measurement, the authors argued that the  $(p, n)$  data should be preferred over the <sup>40</sup>Ti  $\beta$  decay data for calculations of CC ν*<sup>e</sup>* absorption cross sections on argon. Rather than attempt to adjudicate between the conflicting datasets, I have opted to allow each of the three measurements to be used as a source of  $B(GT)$  values in MARLEY cross-section calculations.

#### **B. Extension to higher excitation energies**

Beyond the maximum excitation energy of about 8 MeV probed by the experiments mentioned in the previous section, the presence of additional Gamow-Teller strength is predicted by the model-independent Ikeda sum rule [\[68\]](#page-20-0). This rule states that the summed GT strength  $S_{GT}^-$  ( $S_{GT}^+$ ) over all possible nuclear final states for CC  $v_e$  ( $\bar{v}_e$ ) absorption satisfies the relation

$$
\Delta S_{\text{GT}} \equiv S_{\text{GT}}^- - S_{\text{GT}}^+ = 3 g_A^2 (N_i - Z_i), \tag{36}
$$

where  $N_i = 22$  ( $Z_i = 18$ ) is the neutron (proton) number of the initial  $^{40}$ Ar nucleus. Eq. (36) implies a minimum possible value of  $S_{GT}^-$  = 12  $g_A^2 \approx 19$  for the integrated GT strength associated with the reaction <sup>40</sup>Ar( $v_e$ ,  $e^{-}$ )<sup>40</sup>K<sup>\*</sup>. Comparing this

<span id="page-5-0"></span>



<sup>a</sup>Parenthesized values are based on weak arguments [\[66\]](#page-20-0).

<sup>b</sup>The data tabulated in Ref. [\[58\]](#page-20-0) were multiplied by  $g_A^2 = 1.26^2$  to obtain the *B*(GT) values shown here. <sup>c</sup>A puclear level with parity  $\Pi$  and spin *I* has *natural parity* if  $\Pi = (-1)^J$  Otherwise, it has *unnatural* 

<sup>c</sup>A nuclear level with parity  $\Pi$  and spin *J* has *natural parity* if  $\Pi = (-1)^J$ . Otherwise, it has *unnatural parity*.

<sup>d</sup>Another candidate <sup>40</sup>K level for this transition has  $E_x = 3663.88$  keV and  $J^{\pi} = (1^-, 2, 3, 4^+)$ .

<sup>e</sup>This level is the isobaric analog of the <sup>40</sup>Ar ground state.

f Gamow-Teller transitions are assumed for all levels other than the isobaric analog state.

value to the measured total GT strengths listed in the final row of Table I reveals that the majority of the expected GT strength for CC  $v_e$  absorption on <sup>40</sup>Ar is unmeasured and associated with transitions to high-lying, nucleon-unbound states of  ${}^{40}\text{K}$ .

To supplement the experimental measurements with an estimate of the remainder of the GT strength, I rely on a quasiparticle random-phase approximation (QRPA) calculation by Cheoun, Ha, and Kajino [\[69\]](#page-20-0). To avoid double-counting, theoretical GT matrix elements are included with the experimental ones only for excitation energies at which the integrated QRPA GT strength exceeds the experimental total.

# **C. Adopted matrix elements**

Figure [3](#page-7-0) presents three complete sets of allowed <sup>40</sup>Ar(*ν<sub>e</sub>*, *e*−)<sup>40</sup>**K**<sup>\*</sup> nuclear matrix elements prepared as input for MARLEY based on the measurements and QRPA prediction discussed above. The experimental *B*(GT) values are shown as green, red, or blue bars depending on the dataset. The theoretical QRPA *B*(GT) values are shown in violet.

In addition to extracting GT strengths, both  $\beta$  decay experiments measured values of the Fermi matrix element  $B(F)$ . Under the approximation that isospin is a good quantum number, this matrix element is expected to have the

<span id="page-6-0"></span>

FIG. 1. Gamow-Teller strengths *B*(GT) from two independent measurements of <sup>40</sup>Ti  $\beta$ <sup>+</sup> decay by Liu *et al.* [\[56\]](#page-20-0) and Bhattacharya *et al.* [\[57\]](#page-20-0).

value

$$
B(F) = g_V^2 (N_i - Z_i) = 4
$$
 (37)

and to connect the ground state of  $^{40}$ Ar to a single  $0^+$  isobaric analog state in  ${}^{40}K$ , which has been identified as the level with excitation energy  $E_x = 4.3837$  MeV. Since the experimental data are fully consistent with these expectations, I adopt the value  $B(F) = 4$  for this transition in all three sets of MARLEY matrix elements. The known Fermi transition is represented in each panel of Fig. [3](#page-7-0) by a white bar with horizontal hatch marks. Transitions to all other nuclear levels are assumed to proceed via the Gamow-Teller operator.

Although the differences become important at neutrino energies near threshold, the observables predicted in this paper are largely insensitive to the choice between the three sets of MARLEY matrix elements for the 40Ar(ν*e*, *e*<sup>−</sup>) 40K<sup>∗</sup> reaction. For definiteness, all MARLEY calculations shown in this work (see Sec. [V\)](#page-9-0) are obtained using the ve40ArCC\_Bhattacharya1998.react input file, which contains the matrix elements shown in the middle panel of Fig. [3.](#page-7-0)

# **IV. NUCLEAR DE-EXCITATION MODEL**

To model nuclear de-excitations following CC ν*<sup>e</sup>* absorption on  ${}^{40}Ar$ , I rely on the observation that, due to the selection rules in Eqs. [\(21\)](#page-3-0) and [\(22\)](#page-3-0), each nuclear final state accessed by the neutrino interaction has a well-defined excitation energy, spin, and parity. Distinct treatments are used for bound and unbound nuclear states, with the latter being those for which the excitation energy exceeds the separation energy for at least one nuclear fragment with mass number  $A \leq 4$ . Separation energies are computed in MARLEY using atomic and particle mass data from Refs. [\[70,71\]](#page-20-0). Untabulated atomic masses are estimated using the liquid drop model of Myers and Swiatecki [\[72,73\]](#page-20-0). The full de-excitation cascade is treated as a sequence



FIG. 2. Comparison of the Gamow-Teller strengths *B*(GT) measured using  ${}^{40}$ Ti  $\beta$  decay (see Fig. 1) with those obtained using a measurement of 0◦ (*p*, *n*) scattering by Bhattacharya *et al.* [\[58\]](#page-20-0).

of binary decays while neglecting the possibility of fission and emission of heavy nucleon clusters  $(A \ge 5)$ .

#### **A. Bound states: Discrete level data**

De-excitations of bound nuclear states are handled in MARLEY using a set of nuclear structure data files originally prepared for use with version 1.6 of the TALYS [\[74–76\]](#page-20-0) nuclear reaction code.<sup>1</sup> These in turn are based on the level schemes included in version 3 of the Reference Input Parameter Library (RIPL-3) [\[78\]](#page-20-0). For a large number of nuclei, the files provide tables of discrete nuclear energy levels including their excitation energies, spin-parities, and de-excitation  $\gamma$ -ray branching ratios. Missing experimental measurements

<sup>&</sup>lt;sup>1</sup>The current release of TALYS is version 1.95. However, beginning with TALYS 1.8, some nuclear levels for nuclei with an odd mass number (e.g.,  $^{39}$ K) appear in the structure data files with an unphysical integer spin (as opposed to a half-integer spin). This bug, which remains unfixed [\[77\]](#page-20-0), has prevented updates to the data files distributed with MARLEY.

<span id="page-7-0"></span>

FIG. 3. Complete sets of 40Ar(ν*e*, *e*<sup>−</sup>) 40K<sup>∗</sup> allowed approximation matrix elements distributed as part of MARLEY 1.2.0. The name of the data file in which each set of matrix elements may be found is given in the appropriate legend heading. The QRPA *B*(GT) strengths (violet) were calculated by Cheoun *et al.* [\[69\]](#page-20-0). Citations for the experimental  $B(GT)$  strengths are given in the captions for Figs. [1](#page-6-0) and [2.](#page-6-0)

of these quantities are supplemented by theoretical estimates. Although internal conversion coefficients are provided in the TALYS data files, this process is neglected in MARLEY 1.2.0. In the unusual case where discrete level data are not available for a particular nuclide,  $\gamma$ -ray emission is simulated in the same manner as for unbound nuclear states.

The TALYS structure data files are used with minor reformatting for all nuclides except  ${}^{40}$ K. To ensure consistency with the level assignments made in Sec. [III A,](#page-4-0) I prepared an original decay scheme for  ${}^{40}$ K using the experimental data in Ref. [\[64\]](#page-20-0), the TALYS 1.6 structure file, and (where needed) estimated  $\gamma$ -ray branching ratios computed using the strength function defined in Sec. [IV B 3.](#page-8-0)

#### **B. Unbound states: Statistical emission**

The MARLEY approach to modeling de-excitations of unbound nuclear states rests on the assumption of *compound nucleus* formation: The neutrino interaction leaves the nucleus in a state of thermal equilibrium which de-excites independently of the manner in which it was formed. The number of open decay channels is taken to be large enough that competition between them can be modeled statistically. That is,

transitions to individual nuclear final states can be neglected in favor of averaging over many states of approximately the same energy [\[79\]](#page-20-0). This last assumption is not strictly true for excitation energies slightly above the lowest fragment emission threshold. In such cases it is adopted as an approximation.

Compound nucleus modeling is a key ingredient in nuclear reaction codes designed to compute nucleon-nucleus and nucleus-nucleus cross sections, such as TALYS, EMPIRE  $[80]$ , CCONE  $[81]$ , and CoH<sub>3</sub>  $[82]$ . The treatment in MARLEY uses the Hauser-Feshbach formalism [\[83\]](#page-21-0) common to these other codes.

# *1. Differential decay widths*

For the present application to neutrino-induced deexcitations, the physics content of the Hauser-Feshbach statistical model (HFSM) may be conveniently summarized by the differential decay widths

$$
\frac{d\Gamma_a}{dE'_x} = \frac{1}{2\pi \rho_i(E_x, J, \Pi)} \sum_{\ell=0}^{\infty} \sum_{j=|\ell-s|}^{\ell+s} \sum_{J'=|J-j|}^{J+j} \times T_{\ell j}(\varepsilon) \rho_f(E'_x, J', \Pi') \tag{38}
$$

and

$$
\frac{d\Gamma_{\gamma}}{dE'_{x}} = \frac{1}{2\pi \rho_{i}(E_{x}, J, \Pi)} \sum_{\lambda=1}^{\infty} \sum_{J'=|J-\lambda|}^{J+\lambda} \sum_{\Pi' \in \{-1, 1\}} \times T_{\chi_{\lambda}}(E_{\gamma}) \rho_{f}(E'_{x}, J', \Pi').
$$
\n(39)

which describe de-excitations of a compound nuclear state via emission of a fragment  $a$  or a  $\gamma$  ray, respectively.

Here the initial (final) nucleus has excitation energy  $E_x$  $(E'_x)$ , total spin *J* (*J'*), and parity  $\Pi$  ( $\Pi'$ ); *s*,  $\ell$ , and *j* are the spin, orbital, and total angular momentum quantum numbers of the emitted fragment;  $\rho_i$  ( $\rho_f$ ) is the density of nuclear levels in the vicinity of the initial (final) state;  $\varepsilon$  is the total kinetic energy of the final particles in the rest frame of the initial nucleus; and  $E_{\gamma}$  is the energy of the emitted  $\gamma$  ray. For decays involving emission of a fragment with parity  $\pi_a$ , the value of  $\Pi'$  is fixed by conservation of parity:

$$
\Pi' = (-1)^{\ell} \pi_a \Pi . \tag{40}
$$

The possible  $\gamma$ -ray transitions are labeled by their multipolarity  $\lambda \geq 1$  and by whether they are *electric*  $(X = E)$  or *magnetic*  $(X = M)$  in nature. These two alternatives are distinguished based on the multipolarity and the nuclear parity:

$$
X = \begin{cases} E & \Pi = (-1)^{\lambda} \Pi' \\ M & \Pi = (-1)^{\lambda+1} \Pi' \end{cases}
$$
 (41)

The transmission coefficients  $T_{\ell j}$  and  $T_{X\lambda}$  quantify how likely each decay mode is to occur. The methods used to compute them are described in Secs. [IV B 2](#page-8-0) and [IV B 3.](#page-8-0) For practical calculations, the infinite sums that appear in Eqs. (38) and (39) must be truncated. Because the value of  $T_{\ell i}$  ( $T_{X\lambda}$ ) falls off rapidly with increasing  $\ell$  ( $\lambda$ ), terms beyond  $\ell = \lambda = 5$  are neglected.

The HFSM is often communicated in terms of nuclear scattering cross sections instead of decay widths. To aid the reader <span id="page-8-0"></span>in connecting the expressions given here with more standard presentations (see, e.g., Refs. [\[84,85\]](#page-21-0)), a brief derivation of Eq. [\(38\)](#page-7-0) is provided in Appendix [A.](#page-15-0)

# *2. Fragment transmission coefficients*

The fragment transmission coefficients  $T_{\ell j}$  used in Eq. [\(38\)](#page-7-0) are computed by solving the radial Schrödinger equation (with relativistic kinematics as recommended in Ref. [\[86\]](#page-21-0))

$$
\left[\frac{d^2}{dr^2} + \mathcal{K}^2 - \frac{\ell(\ell+1)}{r^2} - \frac{\mathcal{K}^2}{\varepsilon} \mathcal{U}(r, \varepsilon_{\text{lab}}, \ell, j)\right] u_{\ell j}(r) = 0,
$$
\n(42)

where  $u_{\ell j}$  is the fragment's radial wave function,

$$
\xi = \sqrt{\frac{(2m_a + \varepsilon_{\text{lab}})M'^2 \varepsilon_{\text{lab}}}{(m_a + M')^2 + 2M' \varepsilon_{\text{lab}}}},\tag{43}
$$

is the magnitude of its three-momentum in the rest frame of the initial nucleus, and  $m_a$   $(M')$  denotes the mass of the emitted fragment (final nucleus). The global nuclear optical potential  $U$  developed by Koning and Delaroche  $[86]$  is used in the present calculations. A full description thereof is given in Appendix [C.](#page-17-0)

The quantity

$$
\varepsilon_{\text{lab}} = \frac{\varepsilon^2 + 2\left(m_a + M'\right)\varepsilon}{2M'}\tag{44}
$$

is the fragment's kinetic energy in the rest frame of the final nucleus. The label *lab* is applied to this variable because it also represents the laboratory-frame kinetic energy for the timereversed process in which the fragment is absorbed to form the compound nucleus (see Appendix [A\)](#page-15-0).

The transmission coefficient  $T_{\ell i}$  is related to the energyaveraged *S*-matrix element  $\langle S_{\ell j} \rangle$  via

$$
T_{\ell j} = 1 - |\langle S_{\ell j} \rangle|^2. \tag{45}
$$

The latter quantity may be determined by comparing the full solution  $u_{\ell j}$  of Eq. (42) to the asymptotic form

$$
u_{\ell j}(r) \to \frac{i}{2} [H_{\ell}^-(\eta, \hat{\chi}_r) - \langle S_{\ell j} \rangle H_{\ell}^+(\eta, \hat{\chi}_r)] \tag{46}
$$

valid for large radii  $r$ , where the nuclear optical potential approaches the Coulomb potential. Here  $H^{\pm}_{\ell}$  are the Coulomb wave functions [[\[87\]](#page-21-0), chap. 33]. These depend on the Sommerfeld parameter

$$
\eta \equiv \frac{z Z' \alpha}{\beta_{\text{rel}}},\tag{47}
$$

which is evaluated in terms of the proton number  $z(Z')$  of the emitted fragment (final nucleus) and the relative speed

$$
\beta_{\rm rel} = \frac{\sqrt{\varepsilon_{\rm lab}^2 + 2 \, m_a \, \varepsilon_{\rm lab}}}{m_a + \varepsilon_{\rm lab}} \,. \tag{48}
$$

The numerical techniques used to evaluate the fragment transmission coefficients  $T_{\ell j}$  are documented in Ref. [[\[48\]](#page-20-0), Sec. 2.2.2].

#### *3. γ-Ray transmission coefficients*

The  $\gamma$ -ray transmission coefficients  $T_{X\lambda}$  used in Eq. [\(39\)](#page-7-0) may be written in terms of a strength function  $f_{X\lambda}(E_\gamma)$  such that

$$
T_{X\lambda}(E_{\gamma}) = 2 \pi E_{\gamma}^{2\lambda+1} f_{X\lambda}(E_{\gamma}). \tag{49}
$$

To compute  $\gamma$ -ray strength functions in this work, I adopt the Standard Lorentzian model from RIPL-3 [\[78\]](#page-20-0), which is based on early studies by Brink [\[88\]](#page-21-0) and Axel [\[89\]](#page-21-0). This model assumes that  $\gamma$ -ray emissions of type  $X\lambda$  occur via de-excitation of the corresponding giant multipole resonance, which is parameterized in terms of its centroid excitation energy  $E_{X\ell}$ , width  $\Gamma_{X\ell}$ , and peak cross section  $\sigma_{X\ell}$ . The strength function is evaluated according to

$$
f_{X\lambda}(E_{\gamma}) = \frac{\sigma_{X\lambda}}{(2\lambda+1)\pi^2} \left[ \frac{\Gamma_{X\lambda}^2 E_{\gamma}^{3-2\lambda}}{(E_{\gamma}^2 - E_{X\lambda}^2)^2 + E_{\gamma}^2 \Gamma_{X\lambda}^2} \right], \quad (50)
$$

with the values of the giant resonance parameters given in Table [II.](#page-9-0) Note that some peak cross sections are given in the table in units of mb while Eq.  $(50)$  employs natural units.

#### *4. Transitions to discrete nuclear levels*

The differential decay widths given in Eqs.  $(38)$  and  $(39)$ are appropriate for use at high excitation energies  $E'_x$  where the nuclear levels may be modeled as a continuum. When a discrete level scheme is available for the final-state nuclide, MARLEY uses the excitation energy of the last tabulated level as the lower bound for the continuum. Otherwise, a continuum level density  $\rho_f$  is used all the way down to the ground state  $(E'_x = 0).$ 

Decays to discrete levels of the final-state nucleus are considered by MARLEY in terms of the HFSM partial decay widths

$$
\Gamma_a = \frac{1}{2 \pi \rho_i(E_x, J, \Pi)} \sum_{j=|J-J'|}^{J+J'} \sum_{\ell=|j-s|}^{j+s} \delta_{\pi}^{\ell} T_{\ell j}(\varepsilon) \qquad (51)
$$

and

$$
\Gamma_{\gamma} = \frac{1}{2 \pi \rho_i(E_x, J, \Pi)} \sum_{\lambda = \max(1, |J - J'|)}^{J + J'} T_{X\lambda}(E_{\gamma}). \tag{52}
$$

The symbol  $\delta_{\pi}^{\ell}$ , which enforces parity conservation, is equal to one if Eq. [\(40\)](#page-7-0) is satisfied and zero if it is not. If  $J + J' < 1$ , then the width  $\Gamma_{\gamma}$  vanishes. The expressions in Eqs. (51) and (52) may be derived from Eqs. [\(38\)](#page-7-0) and [\(39\)](#page-7-0) by treating  $\rho_f$  as a δ function centered on the nuclear level of interest.

#### *5. Nuclear level density*

In the continuum, the final level density  $\rho_f$  is computed according to the back-shifted Fermi gas model (BFM) described in Appendix **B**. The initial level density  $\rho_i$  is evaluated according to the BFM at all excitation energies. However, since the overall factor involving  $\rho_i$  cancels out in the evaluation of decay branching ratios, the specific model chosen for  $\rho_i$  does not have any impact on the simulation results.

<span id="page-9-0"></span>TABLE II. Giant resonance parameters used herein for  $\gamma$ -ray strength function calculations. Centroid excitation energies  $E_{X\lambda}$  and widths  $\Gamma_{\chi\lambda}$  are given in MeV. Peak cross sections for electric multipole resonances (σ<sub>*E*λ</sub>) are given in mb, while those for magnetic resonances (σ<sub>*M*λ</sub>) are given in MeV<sup> $-2$ </sup>.



<sup>a</sup>See Ref. [[\[90\]](#page-21-0), p. 129].

 $b$ See Ref. [[\[91\]](#page-21-0), p. 103].

<sup>c</sup>See Ref. [[\[90\]](#page-21-0), p. 132].

 ${}^{d}B_n = 7$  MeV and  $f_{E1}$  is calculated using natural units and the E1 parameters above.

e Default approximation used by version 1.6 of TALYS [\[76\]](#page-20-0).

# **V. RESULTS**

In this section, the MARLEY 1.2.0 implementation of the theoretical models described above is used to obtain predictions of total and differential cross sections for the reaction  $^{40}Ar(v_e, e^-)$ <sup>40</sup>K<sup>∗</sup>. Because MARLEY calculates the four-momentum of every final-state particle for every event, various additional distributions may be studied beyond those presented in this work.

#### **A. Inclusive cross section**

Figure 4 shows MARLEY predictions of the total cross section for inclusive charged-current  $v_e$  absorption on <sup>40</sup>Ar. The important role played by the Coulomb corrections discussed in Sec. [II B](#page-3-0) is illustrated by the different curves in the plot. The default MARLEY approach to Coulomb effects, defined in Eq.  $(25)$ , involves choosing the smaller of two correction factors calculated using the Fermi function and using the MEMA. In Fig. 4, the solid black line gives the cross section calculated using the default approach, while the dotted cyan and dashed red lines give, respectively, the corresponding cross sections obtained when the Fermi function and MEMA are used unconditionally. Applying either correction leads to an enhancement of the total cross section over the uncorrected result, which is drawn as the blue dash-dotted line. The relationships between the different approaches to Coulomb corrections in the present calculation are qualitatively similar to those seen previously using a CRPA model [\[35\]](#page-19-0), but there are some details that are different, e.g., the cross sections calculated using the Fermi function and the MEMA intersect

at a neutrino energy between 50 and 60 MeV, about 10 MeV lower than in the CRPA result.

#### **B. Exclusive cross sections**

Figure [5](#page-10-0) presents the first calculation at supernova energies of total cross sections for exclusive final states in the reaction <sup>40</sup>Ar( $v_e$ ,  $e^{-}$ )<sup>40</sup>K<sup>\*</sup>. Each exclusive channel is labeled in



FIG. 4. Inclusive total cross sections for charged-current absorption of  $v_e$  on <sup>40</sup>Ar. Each curve shows the result obtained using a specific approach to Coulomb corrections.

<span id="page-10-0"></span>

FIG. 5. Exclusive total cross sections for charged-current absorption of  $v_e$  on <sup>40</sup>Ar.

terms of its hadronic content, but zero or more de-excitation  $\gamma$  rays are allowed even when not explicitly listed. Below a neutrino energy of about 10 MeV, only transitions to bound nuclear levels are energetically possible. These de-excite via  $\gamma$ -ray emission. Single neutron emission becomes appreciable around 15 MeV. Although the proton (7.58 MeV) and  $\alpha$  particle (6.44 MeV) separation energies for  ${}^{40}$ K are comparable to the neutron separation energy (7.80 MeV), the Coulomb barrier experienced by these charged particles suppresses their emission relative to neutrons.

Throughout the remainder of this paper, calculations of flux-averaged cross sections will be reported for two distinct sources of low-energy electron neutrinos. The first of these is the approximate supernova neutrino energy spectrum

$$
\phi(E_{\nu}) \propto \left(\frac{E_{\nu}}{\langle E_{\nu} \rangle}\right)^{\alpha} \exp\left[-(\alpha+1)\frac{E_{\nu}}{\langle E_{\nu} \rangle}\right] \tag{53}
$$

described in Ref. [\[92\]](#page-21-0). Here the dependence on the neutrino energy  $E_v$  is expressed in terms of the mean energy  $\langle E_v \rangle$  and a shape parameter  $\alpha$ . Based on an analysis of a simulated supernova, the authors of Ref. [\[92\]](#page-21-0) report values of  $\langle E_v \rangle$  = 14.1 MeV and  $\alpha = 2.67$  for the time-integrated  $v_e$  spectrum, which I denote by  $SN<sub>T</sub>$ . I also consider four instantaneous

TABLE III. Parameters used to compute the supernova neutrino spectrum described in the text. Values of the mean  $v_e$  energy  $\langle E_v \rangle$  and the elapsed time *t* are given in MeV and seconds, respectively. The shape parameter  $\alpha$  is dimensionless.

Configuration	$\langle E_{\nu} \rangle$	$\alpha$	
$SN_{T}$	14.1	2.67	
SN <sub>1</sub>	9		O
$\mathrm{SN}_2$	12	4	0.5
$\mathrm{SN}_3$	15	3.25	3
SN <sub>4</sub>	17	2.9	6.25

spectra estimated using Fig. 1 of Ref. [\[92\]](#page-21-0). These are labeled  $SN<sub>1</sub>$  through  $SN<sub>4</sub>$  in chronological order. Table III gives the values of the spectral parameters and the approximate elapsed time since the start of the supernova for each of these configurations.

The second source of low-energy electron neutrinos considered in this work is the decay

$$
\mu^+ \to e^+ + \nu_e + \bar{\nu}_\mu \,. \tag{54}
$$

For an antimuon decaying at rest  $(\mu\text{DAR})$ , the  $v_e$  energy spectrum is given by [\[93\]](#page-21-0)

$$
\phi(E_{\nu}) \propto E_{\nu}^2 m_{\mu}^{-4} (m_{\mu} - 2E_{\nu}), \qquad (55)
$$

where  $m_{\mu}$  is the muon mass and the neutrino energy  $E_{\nu}$  satisfies

$$
0 < E_\nu < m_\mu/2. \tag{56}
$$

Experimental facilities which generate large numbers of stopped muons, such as the Spallation Neutron Source at Oak Ridge National Laboratory, provide a valuable opportunity to study tens-of-MeV neutrino interactions using a terrestrial source [\[94\]](#page-21-0).

Table [IV](#page-11-0) reports a wide variety of flux-averaged total cross sections for each of the electron neutrino spectra  $\phi(E_v)$  described above. For each entry in the table, the flux-averaged total cross section  $\langle \sigma \rangle_f$  for a specific final state f was obtained via the expression

$$
\langle \sigma \rangle_f = \frac{1}{\Phi} \int \phi(E_\nu) \Bigg[ \sum_L \sigma_L(E_\nu) R_L(f) \Bigg] dE_\nu, \qquad (57)
$$

where

$$
\Phi \equiv \int \phi(E_v) \, dE_v \tag{58}
$$

and the integrals in Eqs.  $(57)$  and  $(58)$  are over the entire neutrino spectrum. Here  $\sigma_L$  is the inclusive total cross section for transitions to a particular  $^{40}$ K nuclear level *L* and  $R_L(f)$  is the branching ratio for the final state  $f$  when the de-excitation cascade begins at the level *L*. The sum in Eq. (57) runs over all energetically accessible nuclear levels. All quantities in Eq. (57) are calculated analytically except for  $R_L(f)$ , which is estimated using Monte Carlo simulations of de-excitations from every nuclear level listed in the MARLEY input file ve40ArCC\_Bhattacharya1998.react. The statis-

<span id="page-11-0"></span>



tical uncertainty associated with each entry in Table IV never exceeds 10% and is typically much smaller.

#### **C. Electron angle and energy distributions**

Figure [6](#page-12-0) shows flux-averaged differential cross sections predicted by MARLEY for the laboratory-frame scattering cosine of the outgoing electron. The upper panel shows the total result (solid black) for the SN*<sup>T</sup>* ν*<sup>e</sup>* spectrum together with the separate contributions arising from Fermi (dashed blue) and Gamow-Teller (dotted red) transitions. The lower panel presents the same quantities for the  $\mu$ DAR  $\nu_e$  spectrum. Competition between the two linear components of the cross section gives rise to a total angular distribution that is nearly flat in both cases, with  $SN<sub>T</sub>$  being slightly forward and  $\mu$  DARslightly backward.

A recent theoretical study [\[36\]](#page-19-0) has pointed out that forbidden nuclear transitions, which are neglected in the present calculation, have an increasingly strong effect on the electron angular distribution as the neutrino energy grows beyond a few tens of MeV. Deviations from the linear behavior shown in Fig. [6](#page-12-0) signal the breakdown of the allowed approximation used by MARLEY. A future measurement of the  $^{40}Ar(v_e, e^-)^{40}K^*$  angular differential cross section will thus provide a powerful constraint on the nuclear modeling needed to predict the relative contributions of the allowed and forbidden transitions.

Figure [7](#page-12-0) shows the flux-averaged differential cross section with respect to the kinetic energy of the outgoing electron. The inclusive prediction for the  $SN_T$  ( $\mu$ DAR) spectrum is shown by the solid black line in the upper (lower) panel, with the other line styles used to represent individual contributions

<span id="page-12-0"></span>

FIG. 6. Flux-averaged differential cross sections with respect to the laboratory-frame scattering cosine  $\cos \theta_e$  of the final-state electron. Top: Calculation for the time-integrated supernova ν*<sup>e</sup>* spectrum described in the text. Bottom: Calculation for  $v_e$  produced by  $\mu^+$ decay at rest.

from four exclusive final states. While the cross sections for both spectra are dominated by de-excitation modes involving only  $\gamma$  rays (loosely dotted blue) or single neutron emission (densely dotted red), the contribution of the latter is much more pronounced for the  $\mu$ DAR case. The small cross sections for single proton and single  $\alpha$  emission are also noticeably enhanced as one moves from the SN*<sup>T</sup>* spectrum to the  $\mu$ DAR spectrum.

# **D. Neutrino energy reconstruction**

The energy of the incident neutrino is distributed among the final products of the <sup>40</sup>Ar( $v_e$ ,  $e^{-}$ )<sup>40</sup>K<sup>\*</sup> reaction according to the relation

$$
E_{\nu} = E_{\text{bind}} + E_e + \mathcal{T}_{\gamma} + \mathcal{T}_{\text{ch}} + \mathcal{T}_n, \tag{59}
$$



FIG. 7. Flux-averaged differential cross sections with respect to the final-state electron kinetic energy  $T_e$ . Top: Calculation for the time-integrated supernova ν*<sup>e</sup>* spectrum described in the text. Bottom: Calculation for  $\nu_e$  produced by  $\mu^+$  decay at rest.

where  $E_e$  is the total energy of the outgoing electron and  $\mathcal{T}_{\gamma}$ ,  $\mathcal{T}_{ch}$ , and  $\mathcal{T}_n$  are, respectively, the total kinetic energies of all deexcitation  $\gamma$  rays, charged hadrons, and neutrons in the final state. The small recoil kinetic energy of the remnant nucleus is included in  $\mathcal{T}_{ch}$ . The change in binding energy  $E_{bind}$  is given by the expression

$$
E_{\text{bind}} = \Delta_{\text{RT}} - m_e + \sum_k m_k + \sum_k Q_k m_e \tag{60}
$$

if electron binding energies are neglected. Here

$$
\Delta_{RT} \equiv m_{\text{atom}}(R) - m_{\text{atom}}(T) \tag{61}
$$

is the difference of ground-state atomic masses between the remnant nucleus (R) and the nuclear target (T =  $^{40}$ Ar),  $m_e$  is the electron mass, and  $m_k$  ( $Q_k$ ) is the mass (electric charge) of the *k*th nuclear de-excitation product. The sums in Eq. [\(60\)](#page-12-0) run over all particles emitted during nuclear de-excitations.

The minimum possible change in binding energy,

$$
E_{\text{bind}}^{\text{min}} \equiv m_{\text{atom}}(F) - m_{\text{atom}}(T) - m_e,
$$
(62)  
=  $m_{\text{atom}}(^{40}\text{K}) - m_{\text{atom}}(^{40}\text{Ar}) - m_e = 0.99 \text{ MeV},$  (63)

occurs for final states in which only  $\gamma$  rays are emitted during nuclear de-excitations. In this case, the nuclide  $F = {}^{40}K$  produced immediately after the primary neutrino interaction and the nuclide *R* remaining after de-excitations are identical.

Since an a priori correction for  $E_{\text{bind}}^{\text{min}}$  may be applied when reconstructing the neutrino energy for any <sup>40</sup>Ar( $v_e$ ,  $e^{-}$ )<sup>40</sup>K<sup>\*</sup> event, Eq. [\(59\)](#page-12-0) may be usefully rewritten in the form

$$
E_{\nu} = E_{\text{bind}}^{\text{min}} + \epsilon_{\text{bind}} + E_e + \mathcal{T}_{\gamma} + \mathcal{T}_{\text{ch}} + \mathcal{T}_n. \tag{64}
$$

Here I have defined the *excess binding energy*

$$
\epsilon_{\text{bind}} \equiv E_{\text{bind}} - E_{\text{bind}}^{\text{min}} \,. \tag{65}
$$

For  ${}^{40}K^*$  de-excitation modes involving only  $\gamma$  rays ( $\gamma$ ), single neutron emission (1*n*), single proton emission (1*p*), or the emission of both a single neutron and a single proton (1*n*1*p*), the excess binding energy takes the values

$$
\epsilon_{\text{bind}}^{\gamma} = 0,\tag{66}
$$

$$
\epsilon_{\text{bind}}^{\text{1n}} = 7.80 \text{ MeV}, \tag{67}
$$

$$
\epsilon_{\text{bind}}^{\text{1p}} = 7.58 \text{ MeV},\tag{68}
$$

$$
\epsilon_{\text{bind}}^{\text{lnlp}} = 14.18 \text{ MeV}. \tag{69}
$$

A useful property of the excess binding energy is that only a few discrete values of this variable are likely to occur at supernova energies. A future analysis of supernova neutrino data may therefore attempt to correct for nonzero values of  $\epsilon_{bind}$  by tagging events in which a nucleon or a heavy fragment was emitted from the struck nucleus.

Beyond the binding energy contributions, the other terms in Eq. (64) vary in the degree to which they may be reconstructed by a detector. In a LArTPC, the primary electron will produce a cm-scale ionization track which may be used to determine its energy and direction. De-excitation  $\gamma$  rays will produce isolated small energy depositions within several tens of cm of the interaction vertex, primarily via Compton scattering on atomic electrons. Reconstruction of both of these features for supernova neutrino interactions is considered in Ref. [\[31\]](#page-19-0), with the conclusion that the energy associated with each can largely be recovered under realistic detector performance assumptions. Neutron tagging and calorimetry, on the other hand, were found to be far more challenging.

Low-energy charged nuclear fragments, such as protons and  $\alpha$  particles, may also produce observable ionizations in a LArTPC. A key challenge for identifying the activity induced by these particles is that, at the energies relevant for supernova neutrinos, charged hadrons will produce mm-scale or smaller ionization tracks. These will likely be difficult to distinguish from the longer track produced by the primary electron. However, if events involving charged nuclear fragment emission can be successfully tagged, perhaps by identifying unusually

large charge deposits near the start of the primary electron track, then at least some of the charged hadron kinetic energy may be recoverable.

To assess the relative importance of the various terms on the right-hand side of Eq. (64), I define several observables, all of which may be interpreted as a reconstructed neutrino energy  $E_v^{\text{reco}}$  under different, often quite optimistic, assumptions. The simplest reconstruction method involves adding the outgoing electron's total energy to the minimum possible change in binding energy for CC ν*<sup>e</sup>* absorption on 40Ar:

$$
E_e^{\text{reco}} \equiv E_{\text{bind}}^{\text{min}} + E_e. \tag{70}
$$

This estimate of the neutrino energy may be refined by adding the summed energies of all de-excitation  $\gamma$  rays

$$
E_{e+\gamma}^{\text{reco}} \equiv E_e^{\text{reco}} + \mathcal{T}_\gamma \tag{71}
$$

and further refined by adding the summed kinetic energies of all final-state charged hadrons

$$
E_{\rm vis}^{\rm reco} \equiv E_{e+\gamma}^{\rm reco} + \mathcal{T}_{\rm ch}.
$$
 (72)

I call the last of these variables the *visible energy* while recognizing that low-energy neutrons may nevertheless produce some observable signals in a LArTPC.

Finally, I consider three possible strategies for implementing a binding energy correction via tagging of final-state nuclear fragments. All three involve conditionally adding one or more terms to the expression for the visible energy above. Under the assumption that de-excitation neutrons may be successfully tagged, I define the reconstructed neutrino energy

$$
E_{\text{tag}}^{n} \equiv E_{\text{vis}}^{\text{reco}} + \delta_{n} \epsilon_{\text{bind}}^{1n} \tag{73}
$$

in which the symbol  $\delta_n$  is defined to be unity when a MARLEY event contains at least one final-state neutron and zero otherwise. Similarly, under the assumption that charged nuclear fragment emission may be successfully identified, I define

$$
E_{\text{tag}}^p \equiv E_{\text{vis}}^{\text{reco}} + \delta_{\text{ch}} \epsilon_{\text{bind}}^{1p} \tag{74}
$$

in which  $\delta_{ch}$  is unity when a MARLEY event contains a charged nuclear fragment in the final state and zero when it does not. In an ideal scenario in which both of these tagging techniques are reliable, a still more refined estimate of the neutrino energy may be obtained via

$$
E_{\text{tag}}^{n+p} \equiv E_{\text{vis}}^{\text{reco}} + \delta_n (1 - \delta_{\text{ch}}) \epsilon_{\text{bind}}^{1n} + \delta_{\text{ch}} (1 - \delta_n) \epsilon_{\text{bind}}^{1p} + \delta_n \delta_{\text{ch}} \epsilon_{\text{bind}}^{1n1p}.
$$
 (75)

Figure [8](#page-14-0) shows the MARLEY prediction for flux-averaged differential sections with respect to each of these observables. The top (bottom) panel of the figure presents results for the  $SN_{T}$  ( $\mu$ DAR) energy spectrum defined earlier. A solid black line is used to draw the differential cross section with respect to the true neutrino energy, while the other line styles represent the various methods for reconstructing it. The  $E_{\text{vis}}^{\text{reco}}$  result is not shown in the top panel since it is difficult to distinguish from the  $E_{e+\gamma}^{\text{reco}}$  one on the scale of the plot.

For both spectra studied, the agreement between the reconstructed and true neutrino energy distributions improves most dramatically as one moves from using only the primary electron  $(E_e^{\text{reco}})$ , thin dashed green) to using both the

<span id="page-14-0"></span>

FIG. 8. Flux-averaged differential cross sections with respect to various definitions of the reconstructed neutrino energy  $E_v^{\text{reco}}$ . Top: Calculation for the time-integrated supernova ν*<sup>e</sup>* spectrum described in the text. Bottom: Calculation for  $v_e$  produced by  $\mu^+$  decay at rest.

electron and the de-excitation  $\gamma$  rays ( $E_{e+\gamma}^{\text{reco}}$ , densely dotted brown) in the reconstruction. Although inclusion of information about charged hadrons is also seen to be helpful, the next most important improvement comes from the inclusion of binding energy corrections related to neutron tagging  $(E_{\text{tag}}^n)$ , thick dashed violet). Due to the higher mean energy of the  $\mu$ DAR spectrum, nuclear fragment emission becomes more important relative to  $SN<sub>T</sub>$ , and the impact of the tagging-based binding energy corrections on neutrino energy reconstruction becomes more pronounced.

To further quantify the performance of each of these energy reconstruction methods, Fig. 9 reports the fractional root-mean-square (rms) resolution

$$
f_{\rm rms}(E_{\nu}) \equiv \sqrt{\left\langle \left( \frac{E_{\nu}^{\rm reco} - E_{\nu}}{E_{\nu}} \right)^2 \right\rangle} \tag{76}
$$



FIG. 9. Fractional rms resolution for the neutrino energy reconstruction methods described in the text.

for each definition of the reconstructed neutrino energy  $E_v^{\text{reco}}$ above. Here, the angle brackets denote the arithmetic mean of the enclosed quantity. The choice of *f*rms as a metric is intended to facilitate comparisons with Fig. 4 of Ref. [\[31\]](#page-19-0) and Fig. 7 of Ref. [\[15\]](#page-19-0), both of which use the same quantity to study energy reconstruction in a full LArTPC detector simulation. The results are shown in small bins of the true neutrino energy  $E_\nu$ . To obtain the curves shown in Fig. 9, a large sample of MARLEY events was generated, and a Monte Carlo estimator for *f*rms was evaluated via

$$
f_{\text{rms}}(E_v \in b) \approx \sqrt{\frac{1}{N_b} \sum_{j=1}^{N_b} \left[ \frac{E_v^{\text{reco}}(j) - E_v(j)}{E_v(j)} \right]^2},\qquad(77)
$$

where the sum runs over over the  $N_b$  simulated events which fell into the neutrino energy bin *b* of interest.

The vertical line seen around 4 MeV for the  $E_e^{\text{reco}}$ curve (thin dashed green) corresponds to the MARLEY energy threshold for CC  $v_e$  absorption. Because the third-forbidden transition between the ground states of <sup>40</sup>Ar ( $J^{\pi} = 0^{+}$ ) and <sup>40</sup>K ( $J^{\pi}$  = 4<sup>-</sup>) is neglected under the allowed approximation, MARLEY predicts a finite resolution for  $E_e^{\text{reco}}$  even at threshold.

The considerable improvements in energy resolution seen between  $E_e^{\text{reco}}$  and  $E_{e+\gamma}^{\text{reco}}$  (densely dotted brown) and between  $E_{e+\gamma}^{\text{reco}}$  and  $E_{\text{tag}}^{n}$  (thick dashed violet) further highlight the conclusions mentioned above with respect to Fig. 8: While ν*<sup>e</sup>* energy reconstruction in CC absorption on argon will benefit from increased information about any final-state particle species, determining the de-excitation  $\gamma$ -ray energies and tagging neutrons are both particularly impactful.

# **VI. SUMMARY AND CONCLUSIONS**

<span id="page-15-0"></span>Due to the potential for DUNE to obtain a once-in-alifetime large-statistics measurement of supernova electron neutrinos, achieving a detailed understanding of tens-of-MeV neutrino-argon interactions is an investment that may yield a high scientific return. This paper expands the ability to model these interactions by providing a first calculation of exclusive cross sections for the <sup>40</sup>Ar( $v_e$ ,  $e^{-}$ )<sup>40</sup>K<sup>\*</sup> reaction at supernova energies. The implementation of the models underlying this calculation in the MARLEY event generator enables studies of neutrino energy reconstruction to be carried out easily. The simple approach pursued in Sec. [V D](#page-12-0) reveals the substantial role that measuring the energies of de-excitation  $\gamma$  rays and (though difficult) neutron tagging may play in optimizing supernova ν*<sup>e</sup>* energy resolution in a future analysis by DUNE. Further insights are available by using MARLEY in conjunction with a realistic detector simulation [\[15,31\]](#page-19-0).

Two major approximations adopted in MARLEY 1.2.0 constitute limitations on the present study that should be revisited in future research. The first of these is the allowed approximation invoked during derivation of the inclusive differential cross section in Sec. [II A.](#page-2-0) In a more detailed calculation of this cross section, the factor  $e^{i\mathbf{q}\cdot\mathbf{x}(n)}$  that appears in the nuclear matrix element from Eq. [\(8\)](#page-2-0) is expanded in a series of multipoles [\[95\]](#page-21-0) that depend on the spherical Bessel function  $j_J(|{\bf q}|r_n)$ , where  $r_n$  is the magnitude of  ${\bf x}(n)$  and *J* is the multipole order. Terms representing forbidden nuclear transitions  $(J > 0)$  vanish in the  $|\mathbf{q}| \to 0$  limit imposed by the allowed approximation, but their contribution to the cross section becomes increasingly important as the momentum transfer grows. Since the centroid energy of the multipole giant resonances grows with *J* roughly like  $41 J A^{-1/3}$  MeV [\[96\]](#page-21-0), the inclusion of forbidden transitions should enhance neutrino scattering to high-lying unbound nuclear states which deexcite primarily via fragment emission. The degree to which this observation affects the present results may be studied in the future by combining a more detailed calculation of the inclusive differential cross section with the MARLEY deexcitation model.

The second major approximation used in this work, which is shared by nearly all calculations of exclusive cross sections for tens-of-MeV neutrino-nucleus scattering, is the compound nucleus assumption discussed in Sec. [IV B.](#page-7-0) Further investigation, both theoretical and experimental, will be needed to clarify the degree to which direct knock-out and preequilibrium processes may safely be neglected in models of low-energy neutrino-nucleus reactions. A key question is how the transition between the compound nucleus picture, which is standard for low-energy neutrinos, and the intranuclear cascade picture, which is commonly used in models of accelerator neutrino interactions, should be handled as a function of neutrino energy.

Although the current discussion has focused specifically on the description of nuclear de-excitations following CC ν*<sup>e</sup>* absorption on  $^{40}$ Ar, the model presented in Sec. [IV](#page-6-0) is sufficiently general that it may be applied unaltered in a variety of other contexts. A natural next step is the use of MARLEY together with an inclusive description of inelastic neutralcurrent scattering on argon, a process for which de-excitations provide the only experimental observables apart from nuclear recoil. While measurements of tens-of-MeV neutrino-argon inelastic cross sections must be pursued to meet the needs of the DUNE supernova neutrino program, more immediate opportunities for confronting MARLEY with data may become available if the code is used to obtain predictions for other nuclei. Near-future measurements that could provide a detailed test of MARLEY include studies of CC ν*<sup>e</sup>* absorption on carbon by JSNS<sup>2</sup> [\[33\]](#page-19-0) and neutrino-induced neutron production on lead, iron, and copper by COHERENT [\[97\]](#page-21-0). Measurements of exclusive cross sections and decay rates for processes that are closely related to neutrino interactions, such as electron-nucleus scattering [\[45\]](#page-19-0) and muon capture [\[98,99\]](#page-21-0), may also provide helpful model constraints. Finally, the capabilities of MARLEY may prove useful in simulating nuclear de-excitations induced by processes beyond the Standard Model, including nucleon decay [\[100,101\]](#page-21-0) and the absorption of fermionic dark matter [\[102,103\]](#page-21-0).

#### **ACKNOWLEDGMENTS**

I thank Myung-Ki Cheoun for providing the QRPA matrix elements used in this work, and I am grateful to the TALYS authors for the decision to release their nuclear structure data files under the terms of the GNU General Public License. Robert Svoboda, Ramona Vogt, and Michael Mulhearn provided helpful feedback on the doctoral thesis [\[34\]](#page-19-0) that was a precursor to this publication. I gratefully acknowledge financial support while at the University of California, Davis, from the John Jungerman-Charles Soderquist Graduate Fellowship and from the DOE National Nuclear Security Administration through the Nuclear Science and Security Consortium under Award No. DE-NA0003180. This manuscript has been authored by Fermi Research Alliance, LLC under Contract No. DE-AC02-07CH11359 with the US Department of Energy, Office of Science, Office of High Energy Physics. The highstatistics MARLEY calculations reported herein were performed using resources provided by the Open Science Grid, which is supported by the National Science Foundation and the US Department of Energy's Office of Science.

# **APPENDIX A: DECAY WIDTH FOR FRAGMENT EMISSION**

In this Appendix, I give a brief derivation of the expression in Eq. [\(38\)](#page-7-0) for the nuclear fragment emission differential decay width of a compound nucleus. A similar approach can be used to obtain the result in Eq. [\(39\)](#page-7-0) for  $\gamma$ -ray emission. The argument presented here is a modern version of one originally given by Weisskopf in Ref. [\[79\]](#page-20-0).

Consider the decay process  $i \rightarrow a + f$  in which a compound nucleus *i* emits a fragment *a* to become a final-state nucleus  $f$ . Adopt the same notation as in Sec. [IV B 1:](#page-7-0) the initial (final) nucleus has spin  $J (J')$ , parity  $\Pi (\Pi')$ , and mass *M* (*M* ). The emitted fragment has spin *s*, orbital (total) angular momentum  $\ell$  (*j*), three-momentum magnitude  $k$ , mass  $m_a$ , and parity  $\pi_a$ . Denote the initial nuclear excitation energy by  $E_x$ , and let the final nuclear excitation energy lie on the

<span id="page-16-0"></span>small interval  $[E'_x, E'_x + dE'_x]$ . The symbol  $\rho_i(\rho_f)$  denotes the spin-parity dependent level density (see Appendix  $B$  2) in the vicinity of  $E_x(E'_x)$  for the initial (final) nucleus.

Within an arbitrary volume *V* and in the rest frame of the initial nucleus, the number of states  $n_{a+f}$  that may be populated by the decay is given by

$$
n_{a+f} = n_a n_f, \tag{A1}
$$

where

$$
n_a = (2s+1)\frac{V}{2\pi^2} \kappa^2 \left| \frac{d\kappa}{dE'_x} \right| dE'_x, \tag{A2}
$$

and

$$
n_f = (2J' + 1) \rho_f(E'_x, J', \Pi') dE'_x.
$$
 (A3)

By detailed balance, the decay width  $\Gamma_{a+f}$  is related to the width  $\Gamma_i$  of the time-reversed absorption process  $a + f \rightarrow i$ via

$$
\Gamma_{a+f} = \frac{n_{a+f}}{n_i} \Gamma_i,
$$
\n(A4)

where

$$
n_i = (2J + 1) \rho_i(E_x, J, \Pi) \frac{dE_x}{dE'_x} dE'_x \tag{A5}
$$

is the number of states in which the compound nucleus *i* may be formed. The absorption width may be written as

$$
\Gamma_i = \phi \sigma,\tag{A6}
$$

where

$$
\phi = \frac{M\,\mathcal{K}}{V\,E_a E_f} = \frac{1}{V} \frac{dE_x}{d\mathcal{K}} \tag{A7}
$$

is the particle flux and

$$
\sigma = \frac{\pi (2J+1)}{\xi^2 (2s+1)(2J'+1)} \sum_{\ell=0}^{\infty} \sum_{j=|\ell-s|}^{\ell+s} T_{\ell j}(\epsilon) \tag{A8}
$$

is the compound nucleus formation cross section. Here  $E_a$  $(E_f)$  is the total energy of the emitted fragment (final nucleus) and

$$
\epsilon = M - m_a - M' \tag{A9}
$$

is the total kinetic energy of the  $a + f$  system. A derivation of the expression in Eq.  $(A8)$  is given<sup>2</sup> in Ref. [\[34\]](#page-19-0). Similar derivations can also be found in, e.g., Refs. [\[84,85\]](#page-21-0).

Combining the results above and summing over the allowed values of *J* , which satisfies the triangle relation

$$
|J-j| \leqslant J' \leqslant J+j,\tag{A10}
$$

leads immediately to Eq. [\(38\)](#page-7-0).

# **APPENDIX B: LEVEL DENSITY MODEL**

The nuclear level density model used in the present calculations is the RIPL-3 parametrization [\[78\]](#page-20-0) of the BFM, which is based on the work of Koning, Hilaire, and Goriely [\[73\]](#page-20-0). The "back shift" used by this model, which accounts for nucleon pairing effects, involves replacing the nuclear excitation energy  $E_x$  by an effective value  $U$  defined by

$$
U \equiv E_x - \Delta, \tag{B1}
$$

where the energy shift

$$
\Delta = \chi_{\text{pair}} \frac{12 \text{ MeV}}{\sqrt{A}} + \delta \tag{B2}
$$

is adjusted to fit experimental data using the empirical parameter  $\delta$ . The pairing factor  $\chi_{\text{pair}}$  is defined by

$$
\chi_{\text{pair}} \equiv \begin{cases} 1 & \text{even-even} \\ 0 & \text{odd-A} \\ -1 & \text{odd-odd} \end{cases} . \tag{B3}
$$

#### **1. Total level density**

Under the BFM, the total density of nuclear levels near excitation energy  $E_x$  is given by the expression [\[73\]](#page-20-0)

$$
\rho(E_x) = \left[\frac{1}{\rho_F(E_x)} + \frac{1}{\rho_0(E_x)}\right]^{-1},
$$
 (B4)

where

$$
\rho_F(E_x) \equiv \frac{1}{\sqrt{2\pi}\sigma} \frac{\sqrt{\pi}}{12} \frac{\exp(2\sqrt{a_{\text{LD}}U})}{a_{\text{LD}}^{1/4} U^{5/4}} \tag{B5}
$$

is the Fermi gas level density and

$$
\rho_0(E_x) = \frac{a_{\text{LD}}}{12 \sigma} \exp(a_{\text{LD}} U + 1) \tag{B6}
$$

is a correction intended to suppress the unphysical divergence of  $\rho_F(E_r)$  at low excitation energies.

Although a constant value for the level density parameter  $a<sub>LD</sub>$  is sometimes used, I adopt the energy-dependent functional form [\[104\]](#page-21-0) recommended by RIPL-3 to correct for the damping of shell effects at high excitation energies:

$$
a_{\text{LD}} \equiv a_{\text{LD}}(E_x, Z, A)
$$
  
=  $\tilde{a}(A) \left\{ 1 + \frac{\delta W(Z, A)}{U} [1 - \exp(-\gamma U)] \right\}.$  (B7)

Here  $\delta W(Z, A)$  is the shell correction energy,  $\tilde{a}(A)$  is the asymptotic value of  $a_{LD}$  at high excitation energies, and  $\gamma$  is a damping parameter that represents how quickly  $a_{LD}(E_x, Z, A)$ approaches  $\tilde{a}(A)$ . The values of these three parameters are

<sup>&</sup>lt;sup>2</sup>Note that there is a misprint in Eqs.  $(A.5)$  and  $(A.6)$  from Ref. [\[34\]](#page-19-0). The quantities  $\ell \pm s_A$ ,  $\ell' \pm s_B$ , and  $\ell \pm s_b$  should be replaced wherever they occur with, respectively,  $j \pm s_A$ ,  $j' \pm s_B$ , and  $\ell' \pm s_b$ .

<span id="page-17-0"></span>
$$
\delta W(Z, A) = \delta M_{\text{exp}}(Z, A) - \delta M_{\text{LDM}}(Z, A), \quad (B8)
$$

$$
\tilde{a} = \alpha A + \beta A^{2/3},\tag{B9}
$$

$$
\gamma = \gamma_0 A^{-1/3},\tag{B10}
$$

where  $\delta M_{\text{exp}}(Z, A)$  is the measured nuclear mass excess [\[71,](#page-20-0)[105\]](#page-21-0) for the nuclide with proton number *Z* and mass number *A*, and  $\delta M_{\text{LDM}}(Z, A)$  is the corresponding prediction for the nuclear mass excess using the liquid drop model [[\[78\]](#page-20-0), p. 3164] [\[72](#page-20-0)[,106\]](#page-21-0).

This work uses the global "BFM effective" values of the empirical parameters  $\alpha$ ,  $\beta$ ,  $\delta$ , and  $\gamma_0$  obtained in Ref. [\[73\]](#page-20-0) using fits to nuclear level data:

$$
\alpha = 0.0722396 \text{ MeV}^{-1}
$$
  $\beta = 0.195267 \text{ MeV}^{-1}$ , (B11)

$$
\gamma_0 = 0.410289 \text{ MeV}^{-1}
$$
  $\delta = 0.173015 \text{ MeV}.$  (B12)

#### **2. Spin dependence**

The density of nuclear levels  $\rho(E_x, J, \Pi)$  with total spin *J* and parity  $\Pi$  near excitation energy  $E_x$  may be written in the form

$$
\rho(E_x, J, \Pi) = \pi(E_x, J, \Pi) R(E_x, J) \rho(E_x),
$$
 (B13)

where  $R(E_x, J)$  is the nuclear spin distribution and  $\pi(E_x, J, \Pi)$  is the parity distribution.

Under the assumption that the individual nucleon spins are pointing in random directions, it can be shown [\[107\]](#page-21-0) that the spin distribution  $R(E_x, J)$  is given by [\[73\]](#page-20-0)

$$
R(E_x, J) = \frac{2J + 1}{2\sigma^2} \exp\left[-\frac{(J + \frac{1}{2})^2}{2\sigma^2}\right].
$$
 (B14)

The spin cutoff parameter  $\sigma$  determines the width of  $R(E_x, J)$ . To calculate this parameter, I adopt the expression recommended by RIPL-3 [\[78\]](#page-20-0) in the absence of discrete level data:

$$
\sigma^{2} = \sigma^{2}(E_{x})
$$
\n
$$
= \begin{cases}\n\sigma_{d, \text{global}}^{2} + \frac{E_{x}}{S_{n}} \big[ \sigma_{F}^{2}(S_{n}) - \sigma_{d, \text{global}}^{2} \big] & \text{for } E_{x} < S_{n} \\
\sigma_{F}^{2}(E_{x}) & \text{for } E_{x} \geq S_{n} \\
\text{(B15)}\n\end{cases}
$$

Here  $S_n$  is the neutron separation energy,

$$
\sigma_F^2(E_x) \equiv (0.01389 \,\text{MeV}^{-1}) \frac{A^{5/3}}{\tilde{a}} \sqrt{a_{\text{LD}} U} \,, \tag{B16}
$$

and

$$
\sigma_{d,\text{global}} \equiv 0.83 \, A^{0.26} \,. \tag{B17}
$$

#### **3. Parity dependence**

Most level density calculations assume equipartition of parity, i.e.,

$$
\pi(E_x, J, \Pi) = \frac{1}{2}.
$$
 (B18)

I adopt this assumption in agreement with RIPL-3. However, I note that more sophisticated treatments of  $\pi$ (*E<sub>x</sub>*, *J*, Π) have been proposed (see, e.g., Ref. [\[108\]](#page-21-0)).

# **APPENDIX C: OPTICAL POTENTIAL**

For the statistical model calculations reported here and implemented in MARLEY, the global nuclear optical potential developed by Koning and Delaroche [\[86\]](#page-21-0) has been adopted. This phenomenological potential is based on fits to nucleonnucleus scattering data and may be written in the form

$$
\mathcal{U} = -\mathcal{V}_V - i\,\mathcal{W}_V - i\,\mathcal{W}_D + d_{\ell s}\,(\mathcal{V}_{SO} + i\,\mathcal{W}_{SO}) + \mathcal{V}_C \,.
$$
 (C1)

Here

$$
d_{\ell s} \equiv j(j+1) - \ell(\ell+1) - s(s+1). \tag{C2}
$$

is the eigenvalue of the spin-orbit operator  $2\ell \cdot s$  for a projectile with definite total angular momentum *j*, orbital angular momentum  $\ell$ , and spin *s*.

The Coulomb potential  $V_C$  is taken to be that of a uniformly charged sphere:

$$
\mathcal{V}_C(r) = \begin{cases} \frac{Z z e^2}{2R_C} \left(3 - \frac{r^2}{R_C^2}\right) & r < R_C\\ \frac{Z z e^2}{r} & r \ge R_C \end{cases}
$$
 (C3)

In the expression above,  $r$  is the radial coordinate of the projectile,  $Z(z)$  is the proton number of the target nucleus (projectile),  $e$  is the elementary charge, and  $R_C$  is the Coulomb radius of the nucleus.

#### **1. Nucleon projectiles**

The volume  $(V)$ , surface  $(D)$ , and spin-orbit  $(SO)$  terms of the optical potential are functions that may be expressed as the product of an energy-dependent well depth and an energyindependent radial part:

$$
\mathcal{V}_V = V_V(\varepsilon_{\text{lab}}) f(r, R_V, a_V), \tag{C4}
$$

$$
W_V = W_V(\varepsilon_{\text{lab}}) f(r, R_V, a_V), \tag{C5}
$$

$$
\mathcal{W}_D = -4 \, a_D^{\mathcal{H}} W_D(\varepsilon_{\text{lab}}) \, \frac{d}{dr} f(r, R_D, a_D^{\mathcal{H}}), \tag{C6}
$$

$$
V_{\text{SO}} = V_{\text{SO}}(\varepsilon_{\text{lab}}) \frac{1}{m_{\pi}^2 r} \frac{d}{dr} f(r, R_{\text{SO}}, a_{\text{SO}}), \tag{C7}
$$

$$
\mathcal{W}_{\text{SO}} = W_{\text{SO}}(\varepsilon_{\text{lab}}) \frac{1}{m_{\pi}^2 r} \frac{d}{dr} f(r, R_{\text{SO}}, a_{\text{SO}}). \tag{C8}
$$

Here  $m_{\pi}$  is the mass of a charged pion, and the well depths  $V_V$ ,  $W_V$ , etc., are real-valued functions of the laboratory kinetic energy  $\varepsilon_{lab}$  of the projectile.

The radial dependence in Eqs.  $(C4)$ – $(C8)$  is given by the Woods-Saxon [\[109\]](#page-21-0) shape

$$
f(r, R, a) = (1 + \exp[(r - R)/a])^{-1}
$$
 (C9)

with effective radius *R* and diffuseness parameter *a*. Table [V](#page-18-0) lists the values of the parameters needed to compute the radially dependent parts of the nuclear optical potential. Each effective radius  $R_j$  is related to its tabulated parameter  $r_j$  via

$$
R_j = r_j A^{1/3} \quad j \in \{V, D, SO, C\} \,. \tag{C10}
$$

Note that all parameter values listed in Table  $V$  are given in fm, while the expressions given in the text assume natural units  $(h = c = 1)$ .

<span id="page-18-0"></span>TABLE V. Radial parameters for the global nuclear optical potential defined in Ref. [\[86\]](#page-21-0).



The expressions for the well depths are most conveniently written in terms of

$$
\mathcal{E} \equiv \varepsilon_{\text{lab}} - E_F^{\mathcal{K}},\tag{C11}
$$

the difference between the laboratory-frame kinetic energy of the projectile  $\varepsilon_{\text{lab}}$  and the nuclear Fermi energy  $E_F^{\mathcal{H}}$  for the projectile species  $\mathcal{N} \in \{p, n\}$  of interest:

$$
V_V(\varepsilon_{\text{lab}}) = v_1^{\mathcal{N}} \left( 1 - v_2^{\mathcal{N}} \mathcal{E} + v_3^{\mathcal{N}} \mathcal{E}^2 - v_4^{\mathcal{N}} \mathcal{E}^3 \right) + V_{\text{Coul}}, \quad \text{(C12)}
$$

$$
W_V(\varepsilon_{\text{lab}}) = \frac{w_1^{\mathcal{N}} \mathcal{E}^2}{\mathcal{E}^2 + \left(w_2^{\mathcal{N}}\right)^2},\tag{C13}
$$

$$
W_D(\varepsilon_{\text{lab}}) = \frac{d_1^{\mathcal{N}} \mathcal{E}^2}{\mathcal{E}^2 + (d_3^{\mathcal{N}})^2} \exp(-d_2^{\mathcal{N}} \mathcal{E}), \tag{C14}
$$

$$
V_{\text{SO}}(\varepsilon_{\text{lab}}) = v_{sol}^{\mathcal{H}} \exp(-v_{so2}^{\mathcal{H}} \mathcal{E}), \tag{C15}
$$

$$
W_{\text{SO}}(\varepsilon_{\text{lab}}) = \frac{w_{sol}^{\mathcal{H}} \mathcal{E}^2}{\mathcal{E}^2 + \left(w_{sol}^{\mathcal{H}}\right)^2}.
$$
 (C16)

Here the Coulomb contribution to  $V_V$  is given by

$$
V_{\text{Coul}} \equiv \delta_{p\mathcal{N}} \overline{V}_C v_1^p (v_2^p - 2 v_3^p \mathcal{E} + 3 v_4^p \mathcal{E}^2), \tag{C17}
$$

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where the symbol  $\delta_{p}$ *N* is defined by

$$
\delta_p \chi \equiv \begin{cases} 0 & \mathcal{N} = n \\ 1 & \mathcal{N} = p \end{cases} . \tag{C18}
$$

Tables 10 and 11 from Ref. [\[86\]](#page-21-0) list the parameters needed to calculate the well depths for a nucleon projectile.

### **2. Complex projectiles**

To compute the nuclear optical potential for complex projectiles  $(A > 1)$ , MARLEY implements a superposition model based on a recommendation by Madland [\[110\]](#page-21-0). It is equivalent to the default treatment used by TALYS. Under this approach, the radial optical model parameters for a projectile with mass number *A* and proton (neutron) number *Z* (*N*) are computed by weighting the corresponding parameters for individual nucleons:

$$
r_V = \frac{N r_V^n + Z r_V^p}{A} \quad r_D, r_{SO} \text{ likewise,}
$$
 (C19)

$$
a_V = \frac{N a_V^n + Z a_V^p}{A} \quad a_D, a_{S0} \text{ likewise.} \tag{C20}
$$

The Coulomb radius parameter  $r<sub>C</sub>$  remains unchanged from the nucleon case. The well depths are evaluated according to the relations

$$
V_V(\varepsilon_{\text{lab}}) = N V_V^n(\varepsilon_{\text{lab}}/A) + Z V_V^p(\varepsilon_{\text{lab}}/A), \quad (C21)
$$

$$
W_V, W_D \text{ likewise,}
$$

$$
V_{\text{SO}}(\varepsilon_{\text{lab}}) = \frac{V_{\text{SO}}^n(\varepsilon_{\text{lab}}) + V_{\text{SO}}^p(\varepsilon_{\text{lab}})}{2A},
$$

$$
W_{\text{SO}} \text{ likewise.}
$$
(C22)

In the expressions above, the superscript *n* (*p*) denotes the value of the corresponding quantity for an individual neutron (proton), e.g.,  $V_{\text{SO}}^n(\varepsilon_{\text{lab}})$  is the spin-orbit well depth for a neutron projectile.

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