Realistic shell-model calculations for astrophysically relevant Gamow-Teller distributions

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Abstract. Electron-capture reaction rates on medium-heavy nuclei are a key ingredient to describe the evolution of core-collapse and thermonuclear supernovae. To estimate these rates it is necessary to know the Gamow-Teller strength distributions involved. In this paper we report some preliminary results of the calculations of Gamow-Teller strength distributions for $pf$-shell nuclei performed in the framework of the realistic shell model.

1. Introduction

Nuclear weak interaction processes play a pivotal role in many astrophysical scenarios [1]. As a matter of fact, electron captures (ECs) on medium-heavy nuclei are crucial in both core-collapse (type II) and thermonuclear (Ia) supernovae evolution. It is therefore mandatory to use accurate weak-interaction rates in the astrophysical simulations to get a reliable description of such scenarios. To this end, it is necessary to know reliable Gamow-Teller (GT) transition strength distributions for a large number of nuclei. In principle, one could get these informations from the experiment studying charge-exchange reactions and discrete $\beta$ decays, actually, however, weak interaction processes take place in stellar environment at relatively high temperatures so that transitions from thermally populated excited states have to be taken into account. It is therefore impossible to directly measure a large fraction of the relevant GT strength distributions and one has to resort to theoretical calculations. To this end, it is obviously necessary to introduce a nuclear model to solve the nuclear many-body problem. Fuller, Fowler and Newman were the first in their pioneering papers [2, 3, 4, 5] to estimate the GT contribution to stellar weak interaction rates using an independent particle model and taking into account the available data from $\beta$ decay experiments. Nowadays, the shell model may be considered the model of choice for such kind of calculations, see for instance Refs.[6, 7, 8].

On these grounds, we have performed a realistic shell-model study of the GT properties of some $pf$-shell nuclei that are astrophysically relevant. More precisely, starting from a realistic nucleon-nucleon ($NN$) potential, we have derived an effective shell-model Hamiltonian and consistently an effective GT operator, and we have employed both of them to calculate the GT distribution strengths and compare them with the available data. The paper is organized as follows. In Sec. 2 it is briefly described the theoretical framework of our calculations, while in
Sec. 3 we show and compare with experiment the results we have obtained for the GT properties of some selected \(pf\)-shell nuclei. Some concluding remarks are reported in Sec. 4.

2. Outline of calculations

The starting point of our calculation is provided by the high-precision CD-Bonn \(NN\) potential [9], that is smoothed integrating out its repulsive high-momentum components by way of the so-called \(V_{\text{low}-k}\) approach [10, 11]. In this way we get a softer \(NN\) potential defined up to a cutoff \(\Lambda\), that preserves the physics of the original CD-Bonn interaction. The value of \(\Lambda\) is chosen, as in many of our recent papers [12, 13, 14, 15, 16] equal to 2.6 \(\text{fm}^{-1}\), this value being a trade off between the need of minimizing the role of the missing three-nucleon force (3NF) [15] and that of ensuring the perturbative behavior of the potential. The Coulomb potential is explicitly taken into account in the proton-proton channel.

Introducing the harmonic oscillator (HO) potential \(U\) it is possible to break up the Hamiltonian for a system of \(A\) nucleons as the sum of a one-body term \(H_0\), which describes the independent motion of the nucleons, and a residual interaction \(H_1\):

\[
H = \frac{\sum_{i=1}^{A} p_i^2}{2m} + \sum_{i<j=1}^{A} V_{\text{low}-k}^{ij} = T + V_{\text{low}-k} = (T + U) + (V_{\text{low}-k} - U) = H_0 + H_1 .
\]  

A truncated model space is then defined in terms of the eigenvectors of \(H_0\). To study the GT transition strength distributions of \(pf\)-shell nuclei we employ a model space spanned by the four \(0f_{7/2}, 1p_{3/2}, 1p_{1/2}, 0f_{5/2}\) proton and neutron orbitals outside the doubly-closed \(^{40}\text{Ca}\) core, and we derive an effective shell-model Hamiltonian \(H_{\text{eff}}\), that takes into account the degrees of freedom that are not explicitly included in the shell-model framework.

This is done by resorting to the many-body perturbation theory, an approach that has been developed by Kuo and coworkers through the 1970s [17, 18]. More precisely, we use the well-known \(\hat{Q}\)-box-plus-folded-diagram method [19], where the \(\hat{Q}\) box is defined as a function of the unperturbed energy \(\epsilon\) of the valence particles:

\[
\hat{Q}(\epsilon) = PH_1P + PH_1Q \frac{1}{\epsilon - \hat{Q}HQ} QH_1P ,
\]  

where the operator \(P\) projects onto the model space and \(Q = 1 - P\). In the present calculations the \(\hat{Q}\) box is expanded as a collection of one- and two-body irreducible valence-linked Goldstone diagrams up to third order in the perturbative expansion[20, 21].

Within this framework the effective Hamiltonian \(H_{\text{eff}}\) can be written in an operator form as

\[
H_{\text{eff}} = \hat{Q} - \hat{Q}' \int \hat{Q} + \hat{Q}' \int \hat{Q} \int \hat{Q} - \hat{Q}' \int \hat{Q} \int \hat{Q} + \ldots ,
\]  

where the integral sign represents a generalized folding operation [22], and \(\hat{Q}'\) is obtained from \(\hat{Q}\) by removing first-order terms [23]. Actually, the above expression for \(H_{\text{eff}}\) is finally rewritten in terms of the \(\hat{Q}\) box derivatives, see Ref.[23] for details.

In present calculations, the single-proton and single-neutron energies have been chosen to reproduce the excitation energies of single-particle states in \(^{57}\text{Cu}\) and \(^{49}\text{Ca}\), respectively, and to reproduce the odd-even mass difference around \(^{56}\text{Ni}\) and \(^{48}\text{Ca}\) [24]. Therefore, the two-body matrix elements (TBMEs) are obtained from \(H_{\text{eff}}\) by subtracting its one-body component .

As mentioned before, we want to derive microscopically the effective GT decay operator tailored for the chosen model space. To this end, we resort to the formalism presented by
Suzuki and Okamoto in Ref. [25]. In this way it is possible to derive an effective one-body GT operator including consistently all contributions up to third-order in the perturbative expansion, without resorting to any empirically fitted parameter. All the details of the derivation of the effective GT operator can be found in Ref. [13], where there are also reported the single-particle matrix elements of the proton-neutron effective GT+ and GT operators.

3. Results

It is worth mentioning that there are available the experimental log ft values for a number of individual β decays of nuclei with mass ranging from A=41 to A=50. We have calculated the corresponding theoretical GT matrix elements and show them in Fig. 1, where they are compared with the experimental values [26]. More precisely, we plot in Fig. 1 the experimental versus the theoretical normalized matrix elements $R(GT)$ defined as follows

$$R(GT) = \frac{M(GT)}{W},$$

where W represents the expected total strength, and $M(GT) = [(2J_i + 1)B(GT)]^{1/2}$. It can be seen that most of the theoretical matrix elements are in close agreement with the experimental ones, most of the points being on a straight line forming a $\pi/4$ angle with the x axis.

![Figure 1](image1.png)

**Figure 1.** Theoretical and experimental R(GT), see text for details.

![Figure 2](image2.png)

**Figure 2.** Running sums of the $^{45}$Sc B(GT) strengths as a function of the excitation energy.

From the experimental point of view, the GT strength distribution can be extracted from the GT component of the charge-exchange-reaction cross section at zero degree, following the standard approach in the distorted-wave Born approximation (DWBA) [27, 28]:

$$\frac{d\sigma^{GT}(0^\circ)}{d\Omega} = \left(\frac{\mu}{\pi\hbar^2}\right)^2 \frac{k_f}{k_i} N_0^{\sigma\tau} |J_{\sigma\tau}|^2 B(p, n),$$

where $N_0^{\sigma\tau}$ is the distortion factor, $|J_{\sigma\tau}|$ is the volume integral of the effective NN interaction, $k_i$ and $k_f$ are the initial and final momenta, respectively, and $\mu$ is the reduced mass.

Therefore we can compare the calculated running sums of the GT strengths ($\Sigma B(p, n)$), obtained with the effective GT operator, with the available data extracted from experiment.

The theoretical GT strength is defined as follows:

...
where indices $i, f$ refer to the parent and grand-daughter nuclei, respectively, and the sum is over all interacting nucleons.

In Fig. 2,3,4 we report the calculated running sums of the GT strengths as a function of the excitation energy for the three nuclei $^{45}$Sc, $^{48}$Ti, and $^{54}$Fe, and compare them with the experiment, and with the shell-model results obtained using the phenomenological interaction KB3G with a quenching factor for the GT operator equal to 0.74.

![Figure 3. Running sums of the $^{48}$Ti B(GT) strengths as a function of the excitation energy.](image)

![Figure 4. Running sums of the $^{54}$Fe B(GT) strengths as a function of the excitation energy.](image)

From the inspection of the figures, it can be seen that our GT strength distributions are in a quite good agreement with the experimental ones, without the need of introducing any “ad hoc” quenching parameter.

4. Concluding remarks
The results that we have reported show that realistic shell-model calculations are able to provide a satisfactory description of the observed GT strength distributions in $pf$-shell nuclei. This approach does not require to introduce any “ad hoc” quenching parameter, thus supporting the reliability and the predictive power of the model.

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