Applications of the USD Hamiltonians to rapid-proton capture rates for sd-shell nuclei

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Abstract. We discuss the use of the USD, USDA and USDB Hamiltonians for calculating rapid-proton capture rates for the sd-shell nuclei. The isobaric-mass-multiplet equation is used to make associations between the levels in the proton-rich nuclei of interest and those in the nuclei with \(N \geq Z\). The theoretical uncertainties associated with the calculated spectroscopic factors and gamma-decay widths are discussed. Results are shown for the \(^{25}\text{Al}(p,\gamma)^{26}\text{Si}\) resonance-capture rate.

1. Introduction

The rapid proton capture (rp-process) is a sequence of proton capture reactions and \(\beta^+\) decays passing through proton-rich nuclei. The rp-process reaction rates are crucial nuclear nuclear physics input to astrophysical models of nucleosynthesis in novae, supernovae and explosive hydrogen burning conditions such as X-ray bursters. A compilation of nuclear structure input and the resulting rates has recently been made [1].

In this paper we will review some applications of nuclear structure theory for the sd-shell for nuclei in the mass region \(A=20-38\). Improved theory input together with new experimental results has greatly reduced the uncertainty for many of the crucial reaction rates. As an example we will show results for the \(^{25}\text{Al}(p,\gamma)^{26}\text{Si}\) resonance-capture rate. In 1995 this rate was uncertain by many orders of magnitude [2]. A combination of theoretical and experimental improvements has reduced this uncertainty to about 30%.

The resonant reaction rate for capture on a nucleus in an initial state \(i\), for an isolated narrow resonances is calculated as a sum over all relevant compound nucleus states \(f\) above the proton-decay threshold [3]

\[
N_A \sigma v >_{\text{res}} i = 1.540 \times 10^{11}\frac{Z}{A} T_9^{-3/2} \sum_f \omega \gamma_{if} e^{-E_{res}/(kT)} \text{cm}^3 \text{s}^{-1} \text{mole}^{-1}. \tag{1}
\]

Here \(T_9\) is the temperature in GigaK, \(E_{res} = E_f - E_i\) is the resonance energy in the center
of mass system, the resonance strengths in MeV for proton capture are

\[ \omega_{\gamma_{if}} = \frac{(2J_f + 1)}{(2J_p + 1)(2J_i + 1)} \frac{\Gamma_{p_{if}}\Gamma_{\gamma_{if}}}{\Gamma_{\text{total}_{if}}}. \]  

(2)

\( \Gamma_{\text{total}_{if}} = \Gamma_{p_{if}} + \Gamma_{\gamma_{if}} \) is the total width and \( J_i, J_p, \) and \( J_f \) are target, the proton projectile \( (J_p = 1/2) \), and states in the final nucleus, respectively. The proton decay width depends on the resonance energy via the single-particle proton width and can be calculated from the proton spectroscopic factor \( C_{i}^{2}S_{if} \) and the single-particle proton width \( \Gamma_{sp_{if}} \) as \( \Gamma_{p_{if}} = C_{i}^{2}S_{if}\Gamma_{sp_{if}} \).

We will discuss the ingredients in this equation in the following sections. In most cases the input comes from a combination of theory and experiment. When this is done the theory has to be good enough so that one can associate a specific final state observed in experiment with a specific theoretical state. The theoretical energy uncertainty is on the order of 150 keV. However, due its exponential dependence in the cross section, it is necessary to know the energies of the individual final states just above the proton-decay threshold to within an uncertainty of about 5 keV. For the proton-rich nuclei in the rp-process path this is achievable in experiments based on transfer reactions or the observation of the protons and gammas in their decay after being formed in beta decay or knockout reactions [4], [5]. But there are often uncertainties in the \( J^\pi \) values. The experimental data for the neutron-rich mirror nucleus is usually known much better (since they lie closer to stability). Thus one tries to make match experimental mirror levels so that information on the \( J^\pi \) value, spectroscopic factors and \( \Gamma_{\gamma} \) from the neutron-rich nucleus can be utilized. The Coulomb displacement energy has state-dependent shifts up to about 300 keV as shown in Fig. (2) for the case of \( ^{26}\text{Mg} \) and \( ^{26}\text{Si} \). Thus when the level density becomes on the order of 300 keV or less the precise matching of mirror states can become ambiguous. We will discuss in Sec. 3 how theory can be used improve the association of mirror levels. In the next section we review the general properties of the sd-shell Hamiltonians and how they have been used to compare with experiment. Finally in Sec. 4 we discuss the cross-section for the \( ^{25}\text{Al}(p,\gamma)^{26}\text{Si} \) example. These results are discussed in more detail [6].

2. sd-shell Hamiltonians

For nearly 30 years the USD Hamiltonian for the \((0d_{5/2}, 0d_{3/2}, 1s_{1/2})\) sd-shell has been used for structure input to rp-process rates. More recently two new Hamiltonians have been obtained from single-valued decomposition (SVD) fits of parameters determined by the 63 two-body matrix and three single-particle energies to a complete set of energy data [7]. The USDA Hamiltonian is based on the SVD fit with 30 linear combinations of parameters and the USDB Hamiltonian is based on 56 linear combinations of parameters.

Comparison of spectroscopic and electromagnetic observables for low-lying states with USD, USDA and USDB has been made [8]. For these low-lying states the comparison of theory vs theory shows that Hamiltonian uncertainty in the spectroscopic factors is on the order of 5%, the B(E2) values on the order of 10% and the B(M1) values on the order of 30%. Comparison of theory vs experiment shows that the theoretical uncertainties are on the order of 20% for spectroscopic factors and 30% for electromagnetic transition strengths.

For \( ^{26}\text{Mg} \) assignments between theory and experiment for about 50 levels in \( ^{26}\text{Mg} \) up to 10 MeV in excitation have been made, based on a comparison of the experimental and theoretical level energies, electromagnetic transition strengths and electron scattering data [9]. These comparisons show that specific experimental and theoretical states can be matched one to one up to about 8 MeV in excitation energy. For the level lifetimes (or \( \Gamma_{\gamma} \) theory and experiment agree within about 30% for levels up to 8 MeV, but there are often large experimental errors for the states above 6 MeV.
3. Mirror level associations

The energies of states in an isobaric multiplet are connected by the isobaric-mass-multiplet equation (IMME):

\[ B(T_z) = a + bT_z + cT_z^2, \]  

(3)

where \( B \) are the binding energies. Ormand and Brown studied the \( b \)- and \( c \)-coefficients of the IMME we use the USD Hamiltonian [10]. They add Coulomb, charge-dependent and charge-asymmetric parts to the nuclear Hamiltonian. For the nuclei considered in [10], \( A=18-22 \) and \( A=34-39 \), the 42 \( b \)-coefficients were reproduced with an rms deviation of 27 keV and the 26 \( c \)-coefficients were reproduced with an rms deviation of 9 keV. There is considerable state-dependence in the \( c \)-coefficients (ranging in values from 130 keV to 350 keV) that is nicely reproduced by the calculations [see Fig. (9) in [10]]. When the only experimental information available is the energy of the neutron-rich nucleus \( B(T_z = T) \), one can use the calculated \( b \)-coefficient to predict the energy of the proton-rich nucleus; \( B(T_z = -T) = B(T_z = T) - 2T_zb_{th} \). This method was used by Herndl et al. [11].

In the example of \( A=26 \), the there is a \( T = 1 \) triplet of states in \( ^{26}\text{Si} \), \( ^{26}\text{Al} \) and \( ^{26}\text{Mg} \). In Fig. (1) values of \( c \) from experiment and theory are compared for \( T = 1 \) states \( A = 26 \) ordered according to increasing experimental energy. The experimental values are obtained for states where all three members of the multiplet are known. In general a good correspondence can be seen, the largest deviations being less than 30 keV. The agreement with experiment and theory [Fig. (1)] for \( A=26 \) appears to be better than obtained in [12] for the odd-odd cases with mass 28, 32 and 36. Predicted binding energies for states in \( ^{26}\text{Si} \) can be then be obtained from Eq. (3), with experimental values of binding energy for corresponding states in \( ^{26}\text{Al} \) and \( ^{26}\text{Mg} \) (when they are known in both) together with the calculated \( c \)-coefficient:

\[ B_{th}^{(26}\text{Si}) = 2B_{exp}^{(26}\text{Al}) - B_{exp}^{(26}\text{Mg}) + 2c_{th}. \]  

(4)

This method was used previously in [12].

Figure 1. \( c \)-coefficients from the isobaric mass multiplet equation versus state number (in order of increasing energy) in \( ^{26}\text{Si} \) based on experimental energies (closed circles) and energies calculated from USDB (open circles).
Figure 2. Experimental excitation energies in $^{26}$Si and $^{26}$Mg [15]. Solid lines are for the states in $^{26}$Si with firm $J^\pi$ values. Dashed lines are for states in $^{26}$Si with uncertain $J^\pi$ values with the most likely mirror associations in $^{26}$Mg with known $J^\pi$ values.

Figure 3. Experimental excitation energies in $^{26}$Si [15] versus predicted energies $E_{th}$ based on Eq. (4). Dashed lines are for states in $^{26}$Si with uncertain $J^\pi$ values with the most likely mirror associations in $^{26}$Mg with known $J^\pi$ values.

Fig. (3) shows the excitation energies for $^{26}$Si obtained from Eq. (4) on the right compared to experiment on the left. The calculated values can then be used as a guide to the correct spin/parity assignments for measured levels in $^{26}$Si. Where no levels in $^{26}$Si are known, levels can be predicted. Two such levels (the $2^+$ and $4^+$) are indicated on the right-hand side of Fig. (3). The energy of the $3^+$ state shown in the right-hand side of Fig. (3) was obtained from the average shift (250 keV) of the five highest states in Fig. (2). Above eight MeV where the property of states in $^{26}$Mg or $^{26}$Al become uncertain we use the energies obtained from the USDB Hamiltonian. This includes the addition of about 170 states with $J^\pi \leq 5^+$ up to 14 MeV in excitation energy.

The three levels that are just above the proton-decay separation energy of 5.51 MeV and of potential importance for the capture reaction at low temperatures are indicated by the arrows in Fig. (3). The $J^\pi$ of levels 16 and 17 are from the recent analysis of Wrede [13] where arguments for the $J^\pi$ are based on all available data for these states. This included the analysis of Bardayan et al. [14] for the $^{28}$Si(p,t) data where an assignment $J^\pi = 2^+$ or $3^+$ was made for state 16. From the associations made in Fig. (3) we can rule out $2^+$.

4. Results for the $^{25}$Al(p,$\gamma$)$^{26}$Si reaction rate

The production mechanism and production site for the long-lived radioactive isotope $^{26}$Al has been of interest since the first indications of $^{26}$Al enrichment in meteoritic inclusions was observed [16]. Understanding its origin would serve as a unique signature for nucleosynthesis in novae and supernovae. The main reaction sequence leading to $^{26}$Al is $^{24}$Mg(p,$\gamma$)$^{25}$Al($\beta^+ + \nu$)$^{25}$Mg(p,$\gamma$)$^{26}$Al.
At the high-temperature conditions expected for shell carbon burning and explosive neon burning the $^{25}\text{Al}(p,\gamma)^{26}\text{Si}$ reaction becomes faster than the $^{25}\text{Al}\beta$ decay. Since $^{26}\text{Si}\beta$ decays to the short-lived $0^+$ state of $^{26}\text{Al}$, the production of the long-lived ($5^+$) state is by-passed. In a recent paper [15] energies of levels in $^{26}\text{Si}$ were measured and used together with previous data and theoretical input to obtain a cross section for the $^{25}\text{Al}(p,\gamma)^{26}\text{Si}$ reaction. An updated theoretical calculation was presented in [6] and is reviewed here.

The total resonance-capture reaction rates have been calculated for each of the interactions USD, USDA and USDB. Fig. (4) shows the results for the resonance-capture rate obtained using the properties of $^{26}\text{Si}$ given in Table I of [6]. The $\Gamma_p$ and $\Gamma_\gamma$ in this case are all based on the USDB Hamiltonian. In Fig. (5) we show some sensitivity studies. The upper two panels (a) and (b) show the results based on $\Gamma_p$ and $\Gamma_\gamma$ from the USDA and USD Hamiltonians relative to USDB. In panel (c) we compare the rate obtained when the theoretical $\Gamma_\gamma^{(26}\text{Si})$ are replaced by $\Gamma_\gamma^{(26}\text{Mg})$ with the excitation energies the same in both cases. These $\Gamma_\gamma$ differ because the electromagnetic matrix elements have a small mirror asymmetry. This comparison shows that at the level of 10% it is adequate to take the $\Gamma_\gamma$ information from the mirror nucleus.

For the region of $\log_{10}(T9) < -0.8$ the resonance-capture rate comes entirely from the 5.675 MeV $1^+$ state (number 15). Since $\Gamma_\gamma >> \Gamma_p$ for this case the rate is determined by $\Gamma_p$. The large change shown on the left-hand side of panels (a) and (b) in Fig. (5) is due to the change in the relatively small spectroscopic factors: 0.0048 (USDB), 0.0027 (USDA) and 0.0035 (USD). For this region of T9 we recommend the USD rate with an uncertainty of 40% coming from the spread of the theoretical spectroscopic factors.

For the region of $-0.7 < \log_{10}(T9) < 0.5$ the rate is dominated by the properties of the $3^+$ state at 5.915 MeV (number 16). Since $\Gamma_\gamma < \Gamma_p$ the rate is determined by $\Gamma_\gamma$. The gamma-decay half-life of the analogue $3^+$ level in the mirror nucleus $^{26}\text{Mg}$ has been measured [17]. Experiment and theory are compared for lower energy states of $^{26}\text{Mg}$ in Table I and Fig. (2) of [9]. The experimental half-life of this $3^+$ level in $^{26}\text{Mg}$ of 14(6) ps [17] is larger than the USDB result of 4.0 ps. The USDA and USD values for the half-life are 4.5 and 5.0 fs, respectively. Based on the comparisons shown in Fig. (2) of [9] for the lifetimes of other levels in $^{26}\text{Mg}$ above five MeV (levels 10-22), this deviation is larger than expected. However, the experimental uncertainty is relatively large for this lifetime. It has only been measured once by the Doppler shift attenuation method [17]. Thus, we choose to use the USDB value. Since Matic et al., [15] use the experimental value, their rate is about a factor lower than ours in this region of temperature. It would be important to improve the experimental uncertainty in this lifetime. In addition, one could measure the gamma-decay decay branching for the 403 keV resonance in $^{26}\text{Si}$ which is predicted to be 3% relative to proton decay. The theoretical uncertainty for this energy range coming from $\Gamma_\gamma$ is about 20%. But one should confirm the experimental result for $^{26}\text{Mg}$ which deviates from the theory outside of this error.

For the region of $0.7 < \log_{10}(T9)$ the rate comes from the contribution of many states with $\Gamma_\gamma << \Gamma_p$. The $\omega_\gamma$ depends on the $(2J_f + 1)$ level density and the associated $\Gamma_\gamma$. The sd-shell provides a fairly realistic model for the positive-parity level density up to 10 MeV, but there will be contributions from pf shell intruder states starting with the possible state at 7.2 MeV in $^{26}\text{Mg}$ [9]. Starting with the known $3^-$ state in $^{26}\text{Mg}$ at 6.8 MeV there will be contributions from negative-parity states. At $\log_{10}(T9)=1$ we estimate that the effective level density and the effective rate is about a factor of two higher than that given by the sd-shell model. Above $\log_{10}(T9) = 1$ one should base the rate on a Hauser-Feshbach formulation with level densities adjusted to match the known level density in the region of 6–9 MeV excitation energy.

The astrophysical implications for novae and x-ray bursts in terms of the competition between the $^{25}\text{Al}(p,\gamma)^{26}\text{Si}$ and the $^{25}\text{Al}\beta$ decay rates is shown in Fig. (9) of [15]. Our factor of three higher rate for $^{25}\text{Al}(p,\gamma)^{26}\text{Si}$ compared to that of [15] in the temperature range of interest, $\log_{10}(T9)=0.1-0.3$, will relatively reduce the population of the long-lived $5^+$ state of $^{26}\text{Al}$.
by bypassing its production. It would be interesting to apply these new rates to various astrophysical scenarios to find the quantitative consequences. For the next generation of rp capture cross section calculations it will be important to consider theoretical errors coming from uncertainties within the model-space assumptions as well as those that come from the limitations of the model-space truncations.

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