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A new approach to estimating the probability for beta-delayed neutron emission

E.A. McCutchan,[1], A.A. Sonzogni,[1] T.D. Johnson,[1] D. Abriola,[2] M. Birch,[3] and B. Singh[3]

[1]*National Nuclear Data Center, Brookhaven National Laboratory, Upton, NY 11973-5000, USA*
[2]*Nuclear Data Section, International Atomic Energy Agency, A-1400 Vienna, Austria*
[3]*Department of Physics and Astronomy, McMaster University, Hamilton, Ontario, Canada*

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P.O. Box 5000
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A new approach to estimating the probability for β-delayed neutron emission

E.A. McCutchan,[1,*] A.A. Sonzogni,[1] T.D. Johnson,[1] D. Abriola,[2] M. Birch,[3] and B. Singh[3]

[1] *National Nuclear Data Center, Brookhaven National Laboratory, Upton, NY 11973-5000, USA*
[2] *Nuclear Data Section, International Atomic Energy Agency, A-1400 Vienna, Austria*
[3] *Department of Physics and Astronomy, McMaster University, Hamilton, Ontario, Canada*

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The probability for neutron emission following β decay, P_n, is a crucial property for a wide range of physics and applications including nuclear structure, r-process nucleosynthesis, the control of nuclear reactors, and the post-processing and handling of nuclear fuel. Despite much experimental effort, knowledge of P_n values is still lacking in very neutron-rich nuclei, requiring predictions from either systematics or theoretical models. Traditionally, systematic predictions were made by investigating the P_n value as a function of the Q value of the decay and the neutron separation energy in the daughter nucleus. A new approach to P_n systematics is presented which incorporates the half-life of the decay and the Q value for the β-delayed neutron emission. This prescription correlates the known data better and thus improves the estimation of P_n values for neutron-rich nuclei. Such an approach can be applied to generate input values for r-process network calculations or in the modeling of advanced fuel cycles.

I. INTRODUCTION

In neutron-rich nuclei, β-decay can populate high-lying states above the neutron separation energy, S_n, in the daughter nucleus. In these cases, the excited levels usually decay via neutron emission, leading to a β-delayed neutron spectrum. For many areas of nuclear science, the fraction of decays that lead to neutron emission, the so-called β-delayed neutron emission probability, P_n, is a critical quantity. P_n values are important for the reactor applications, as it is the flux of these delayed neutrons which is used to control and regulate the reactor, as well as for nuclear waste management [1]. In r-process nucleosynthesis calculations, the P_n values have a direct impact [2, 3] on the predicted abundances, as any β-delayed neutron branch influences the path of the decay back to the valley of stability. Concerning basic nuclear structure, P_n values can also be used to test models of β-decay and provide insight [4] into the microscopic structure of the nuclei involved in the β-decay process.

There are currently just over two hundred nuclei with measured P_n values [5]. However, based on our knowledge of masses, there are over 600 nuclei where β-delayed neutron emission is energetically possible [6]. This gap in measured and potential β-delayed neutron emitters requires the use of theoretical approaches to fill in the holes. There are a wide range of techniques currently used to predict P_n values including phenomenological [7], shell model [8] and macroscopic-microscopic theories [9, 10].

II. TRADITIONAL SYSTEMATICS VIA THE KRATZ HERRMANN FORMULA

The standard method for systematic investigations of P_n values has utilized the so-called Kratz-Herrmann formula (KHF) given by [11]

$$P_n \sim a \left[\frac{Q_{\beta n}}{Q_\beta - C} \right]^b \tag{1}$$

where $Q_{\beta n} = Q_\beta$ - S_n with Q_β the Q value for β decay and S_n the neutron separation energy in the β-decay daughter nucleus. The cutoff parameter C represents the pairing gap and varies depending on the even/odd character of the β-decaying nuclide. On a log-log plot, the KHF would generate a straight line described by the parameters a (intercept) and b (slope).

The KHF has been applied most recently in the work of Pfeiffer *et al.*,[7] which includes a compilation of experimental P_n values in the fission fragment region as well as global Quasi-Random-Phase Approximation (QRPA) calculations for spherical and deformed shapes. There have been significant improvements in our knowledge of the quantities relevant to β-delayed neutron emission since the Pfeiffer work performed in 2002. Masses of neutron rich nuclei have been measured to very high precision owing to the work of Penning traps [12] and storage

* Corresponding author:
mccutchan@bnl.gov

rings [13]. In addition, new radioactive beam facilities have opened up the entire nuclear chart to measurements of P_n values, where in the past such measurements were concentrated in the fission fragment region.

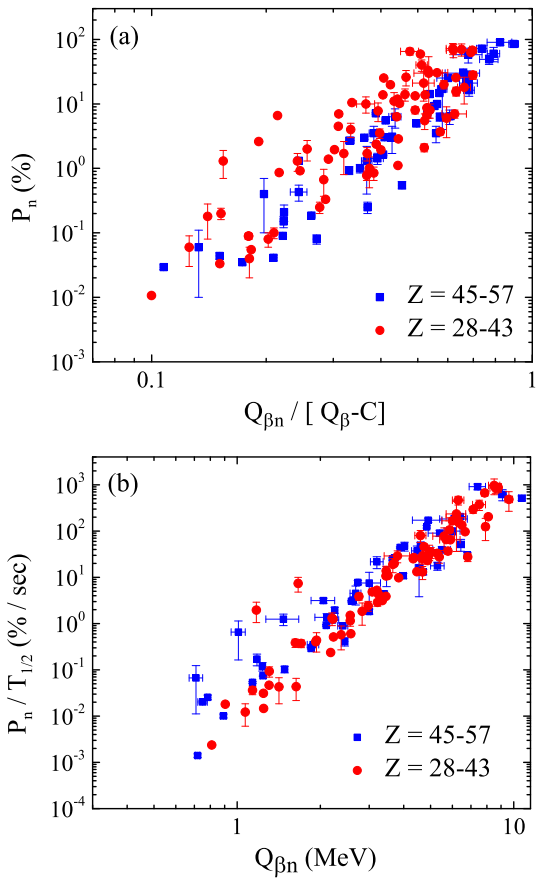

FIG. 1. (Color online) Systematics of P_n values for fission fragments with the heavy and light regions indicated by the blue squares and red circles, respectively. (a) P_n in the traditional systematics form (KHF) given as a function of $Q_{\beta n}/[Q_\beta\text{-}C]$. (b) In the present systematics, $P_n/T_{1/2}$ is given as a function of $Q_{\beta n}$.

Such advancements warrant a new look into the systematics of β-delayed neutron emission probabilities. Figure 1(a) demonstrates the application of the Kratz Herrmann formula to the fission fragment region by plotting the P_n values for nuclei with $28 \leq Z \leq 57$. The heavy and light fission fragment regions are distinguished by the blue squares and red circles, respectively. In the present analysis, P_n and $T_{1/2}$ values are taken from the most recent version of the Nuclear Wallet Cards, combined with data from ENSDF [5]. Q values are taken from the 2011 update to the Atomic Mass Evaluation work of Audi *et al.* [6]. The original Pfeiffer *et al.*, work[7] obtained the fit parameters a=106(38) and b=5.51(61) with a reduced χ^2 of 81 in fitting the light fission fragment region. With the new P_n values and improved masses, a fit to the same region gives a=119(42) and b=5.45(48) with a reduced χ^2 of 146. Within the error bars, the fit parameters are practically identical; the large increase in the reduced χ^2 value can be attributed to the large decrease in uncertainty on the measured Q values. There is some overall linear trend in the data plotted in Fig. 1(a), however, for any given $Q_{\beta n}/[Q_\beta\text{-}C]$ value, the data span generally span two orders of magnitude or more. There is also a suggestion in Fig. 1(a) that the application of the KHF is region dependent, that is, the data for the light fission fragment region appear to follow a trajectory different from that of the heavy fission fragment region.

III. NEW SYSTEMATICS: THE $P_n/T_{1/2}$ RATIO

In order to make reliable predictions for P_n values based on systematics, a more compact group of the data is desirable. A new systematics approach can be motivated by considering the components of P_n given by

$$P_n \sim \frac{\int_{S_n}^{Q_\beta} S_\beta(E) f(Z, Q_\beta - E) dE}{\int_0^{Q_\beta} S_\beta(E) f(Z, Q_\beta - E) dE} \tag{2}$$

where $S_\beta(E)$ is the β decay strength function and $f(Z, Q_\beta - E)$ is the Fermi integral. The denominator of Eq. (2) is simply the inverse of the half-life of the decay. Note that this integral, over the entire Q_β energy window, samples all aspects of the strength function. Particularly in the decay to low-lying states, this can have significant structural effects. Such a structural dependence can be folded into the systematics by considering instead the ratio of the P_n value to the half-life, given by

$$\frac{P_n}{T_{1/2}} \sim \int_{S_n}^{Q_\beta} S_\beta(E) f(Z, Q_\beta - E) dE. \tag{3}$$

This ratio then samples the strength function only in the energy window from S_n to Q_β. This energy regime is usually several MeV above the ground state and is an area of quite high level density, so one expects a rather smoothly varying strength function.

Applying a similar parametrization as the KHF, we consider the systematics of the ratio of the P_n value to the half-life with

$$\frac{P_n}{T_{1/2}} \sim c Q_{\beta n}^d \tag{4}$$

where c and d are free parameters representing the intercept and slope, respectively, when plotted on a log-log scale. The $P_n/T_{1/2}$ ratio is plotted in given Fig. 1(b) for the same nuclei as in Fig. 1(a). In the formalism of Eq. (4), the data coalesce into a much more compact trajectory, compared with the traditional KHF systematics. The scatter in $P_n/T_{1/2}$ is now reduced to an order or

magnitude or less, for a given $Q_{\beta n}$ value. Furthermore, the trend for the heavy and light regions now overlaps, suggesting the present prescription provides a more global description of the data. While only the fission fragment region has been considered here, a compact trajectory for light nuclei (Z <26) can also be obtained when the $P_n/T_{1/2}$ ratio is considered [14].

The more compact trend in the systematics shown in Fig. 1(b) allows for more reliable predictions of P_n to be made using the ratio of P_n to the half life. The reduced χ^2 of the fitting using the $P_n/T_{1/2}$ ratio is much improved compared with the standard KHF approach. For the light fission fragment region it is reduced from 146 to 35, while in the heavy fission fragment region it is reduced from 78 to 55. The parameters obtained in the fits to $P_n/T_{1/2}$ are c=0.0097(9) and d=4.87(7) for the light fission fragments and c=0.016(2) and d=4.55(13) for the heavy fission fragments.

With the data lying on a more compact trajectory, is it easier to identify and highlight those nuclei that deviate from the overall trend. For the light fission fragment region with $28 \leq Z \leq 43$, there are two nuclei (with $Q_{\beta n}$ values between 1 and 2 MeV) which exhibit $P_n/T_{1/2}$ values considerably larger than expected compared with the overall systematics. These outliers correspond to ^{109}Mo and ^{110}Mo; their P_n values have been recently measured in Ref. [15] as 1.3(6)% and 2.0(7)%, respectively. These values can be compared with the predictions from the systematic fit to $P_n/T_{1/2}$ which yields P_n values of 0.01%-0.03%. In the heavy fission fragment region, there are similarly some obvious outliers, with P_n values which appear too large when compared with the systematics. Most apparent are ^{147}Ba and ^{148}Ba, with $Q_{\beta n}$ values of 0.7 MeV and 1.0 MeV, respectively. As evident in Fig. 1(b), these points have substantial error bars (owing to large uncertainty (>50%) in their P_n values) and highlight cases where a remeasurement is needed.

In Fig. 2, the application of the $P_n/T_{1/2}$ ratio to individual isotopic chains is considered for the light fission fragment region. The selected chains span ten units in proton number, however, there is little variation in the trajectories of $P_n/T_{1/2}$. Thus, the systematics in this region suggest there is little or no dependence of either the slope or the intercept on mass or proton number. While the majority of the chains exhibit quite linear trajectories, the Rb isotopes (blue triangles) show an anomalous trend at large $Q_{\beta n}$ values. In particular, the $P_n/T_{1/2}$ ratios for ^{100}Rb and ^{102}Rb deviate from the overall linear behavior of the remainder of the isotopic chain. Given that both nuclei are cases where the P_n value originates from a single measurement and is quoted with substantial uncertainty (P_n=6(3) [16] for ^{100}Rb and P_n=18(8) [17] for ^{102}Rb) new measurements appear warranted.

The quality of the predictions for P_n values using the current approach is illustrated in Fig. 3. The P_n values for the Gallium isotopic chain are calculated using the c and d parameters given above for the light fission fragment region, the $Q_{\beta n}$ values from Audi *et al.,* [6] and the

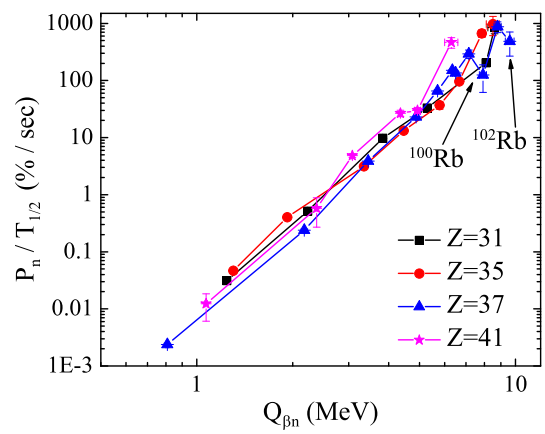

FIG. 2. (Color online) $P_n/T_{1/2}$ plotted as a function of $Q_{\beta n}$ for the Ga (Z=31), Br (Z=35), Rb (Z=37) and Nb (Z=41) isotopic chains. Note the kinks the trajectory for Rb at A=100 and 102.

experimentally measured half-lives. Included for comparison are the QRPA calculations of Moller *et al.,* [9]. With the exception of ^{84}Ga, the $P_n/T_{1/2}$ systematics predict the P_n values to within 30% or better. In the case of ^{84}Ga, the prediction underestimates by more than 50%, a trend also seen in the QPRA calculations.

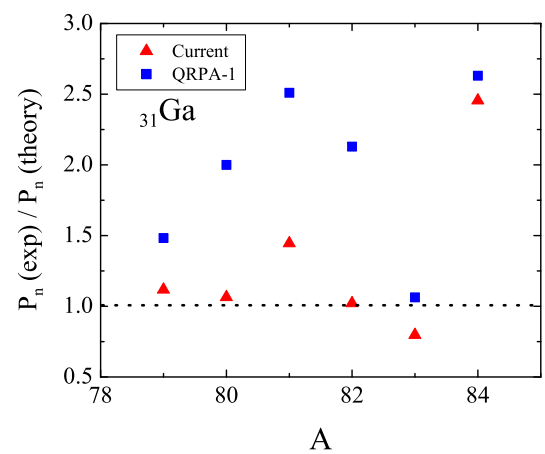

FIG. 3. (Color online) Comparison between experimental P_n values and those predicted by the present analysis and global QPRA calculations [9] for the Gallium isotopes. Plotted is the ratio of the experimental P_n value to the predictions from the different approaches.

In Fig. 4, the $P_n/T_{1/2}$ ratios for sample isotopic chains in the heavy fission fragment region are plotted as a function of $Q_{\beta n}$. For these nuclei, there is still considerable scatter in the overall trajectories. Some anomalous nuclei emerge, for example, the most neutron-rich isotope of La (A=150), where the $P_n/T_{1/2}$ ratio increases rela-

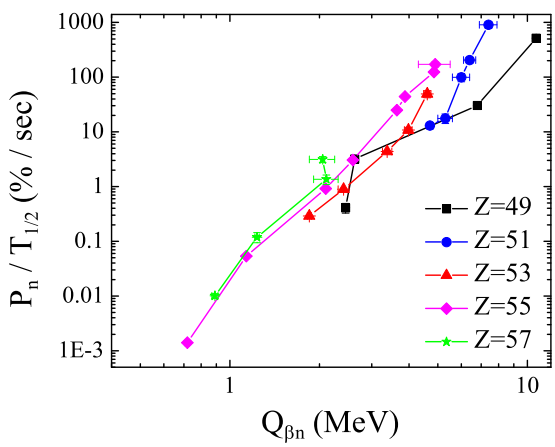

FIG. 4. (Color online) $P_n/T_{1/2}$ plotted as a function of $Q_{\beta n}$ for the In (Z=49), Sb (Z=51), I (Z=53), Cs (Z=55), and La (Z=57) isotopic chains.

tive to the neighbor while the $Q_{\beta n}$ value remains nearly constant. For large $Q_{\beta n}$ values, there is little overlap in trajectory of any of the chains. Note that many of these isotopes are adjacent to the Z=50 major shell. Thus, it is possible that shell effects play a more pronounced role in these nuclei and global systematic investigations may not be applicable. Another explanation for the divergent trajectories for the Z=49 and 50 isotopic chains is the possibility of two neutron emission. For the most neutron rich isotopes of In and Sb, β-delayed two neutron emission is energetically allowed based on the measured Q values. Such a mode has not currently been observed, however, could be entangled in the measured P_n values.

IV. CONCLUSION

Given the importance of P_n values to a wide range of basic and applied sciences, a reliable method for predicting values in unexplored regions of the nuclear chart is desirable. Application of the standard Kratz Herrmann formula, where the P_n value is considered as a function of $Q_{\beta n}/[Q_\beta\text{-}C]$, was shown to exhibit considerable scatter in the data. A new prescription was outlined which considers the ratio of the β-delayed neutron emission probability to the half-life of the decay, $P_n/T_{1/2}$, and its correlation with the allowed Q value for β-delayed neutron emission. This approaches correlated the known data better, providing more accurate estimations of P_n values for nuclei where only the half-life and masses are known. In the light fission fragment region, a remarkable correlation is found which can be used not only for predictions, but also for highlight those nuclei where new measurements are needed. In the heavy fission fragment region, the correlation is less compact, which could point to shell effects around Z=50 or the possible influence of β-delayed two neutron emission.

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