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Improving systematic predictions of beta-delayed neutron emission probabilities

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The probability, P_n, for emitting a neutron following β decay is critical in many areas of nuclear science, from understanding nucleosynethesis during the r-process to control of reactor power levels and nuclear waste management. As it is not always easy to measure or calculate, indirect empirical approaches have been developed to estimate the P_n value from the decay Q_β value and the neutron separation energy, S_n. Here, we present a new prescription incorporating also the half-life, $T_{1/2}$, which correlates the known data better and thus improves an estimation of P_n when only $T_{1/2}$, Q_β, and S_n are known. This new relation can be used to predict P_n values for cases where the half-life is known thus, can be useful in r-process network calculations and in modeling advanced fuel cycles.

PACS numbers:

Electroweak processes can in principle be calculated quite accurately. In super-allowed nuclear β decay, the rates can be calculated [1, 2] to a fraction of a percent, and provide a stringent constraint on the weak-coupling constant. However, these are very special cases where the overlap of the initial and final states is near perfect, and the decay proceeds almost entirely to a single state. In general, the β-decay is fragmented over many states and the decay rate reflects a convoluted summation of the β strength function, $S_\beta(E)$, and the Coulomb-distorted phase space for leptons, $f(Z, Q_\beta)$. In neutron-rich nuclides, of the fraction of β decay that proceeds to high-lying states above the neutron separation energy in the daughter nucleus, S_n, almost all of the fraction immediately decays via neutron emission and leads to a β-delayed neutron spectrum. This spectrum can reveal a great deal about the underlying wave functions involved and hence is interesting for nuclear structure investigations [3, 4]. However, for most applications, like r-process nucleosynthesis network calculations [5, 6] or reactor control and post-processing [7], what is most important is the fraction of decays that lead to a neutron being emitted, the so called β-delayed neutron emission probability, P_n. Accurate knowledge of P_n values can also provide constraints and guidance in developing new models for β decay [8]. One key parameter to any P_n systematics is the phase space available for β-delayed neutron decay, namely the energy window Q_β-S_n. Moving from stability towards the neutron drip line, two effects are seen as a function of the neutron number: an odd-even staggering in both Q_β and S_n coupled with an increase in Q_β and a decrease in S_n. In calculating the $Q_{\beta n}$ value the odd-even staggering tends to cancel out, and since the quadratic increase in Q_β is faster than the decrease in S_n, this leads to a rapid increase of the phase space and the values of P_n rise from a small fraction of a percent just beyond stability to 100% at the dripline.

Numerous theoretical approaches have been utilized to predict P_n values ranging from phenomenological [9] to shell model [10] to macroscopic-microscopic approaches [11]. Recently, very detailed and sophisticated theoretical models have been developed [12, 13], however, these calculations are usually limited to a small mass region. Despite much experimental effort, knowledge of P_n values is sparse and many applications, particularly r-process abundance calculations, must rely heavily on theoretical predictions for basic β-decay properties.

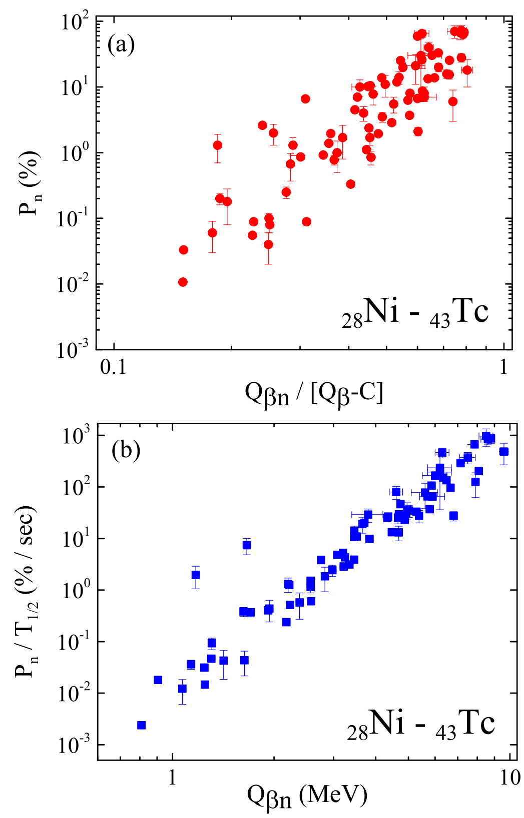

FIG. 1: (Color online) Systematics of P_n values in the region of light fission fragments. (a) P_n plotted as a function of $Q_{\beta n}/[Q_\beta$-C]. (b) $P_n/T_{1/2}$ plotted as a function of $Q_{\beta n}$.

It is the purpose of the present paper to investigate correlations between the currently known values of P_n and other gross properties of β decay, $T_{1/2}$, Q_β, S_n, in order to make reliable predictions for P_n when the value has not been measured. This has been tried before, but we find a better grouping of known data can be obtained by relating the ratio $P_n/T_{1/2}$ to the neutron decay window, $Q_{\beta n}$. A tighter grouping of known data leads to better fit parameters, and thus a more reliable and constrained estimate for unknown P_n values. In the following, we will review previous correlation approaches, present the same data and fits with our new prescription, then discuss why this correlation works so well.

The most recent compilation of P_n values is the work of Pfeiffer *et al.,* [9], completed in 2002. This influential work which included both a systematic study as well as global QRPA calculations for spherical and deformed shapes, is widely used to estimate P_n values in unexplored neutron-rich regions. The Pfeiffer compilation presents a systematic investigation using the so-called "Kratz-Herrmann Formula" (KHF) given by [14]

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

where $Q_{\beta n} = Q_\beta$ - S_n with Q_β and S_n the standard Q value for β decay and the neutron separation energy, respectively. The cut-off parameter, C, represents the pairing-gap which depends on the even/odd character of the β-decaying nuclide. On a log-log plot, Eq. (1) yields a straight line which can be fit with the parameters a (intercept) and b (slope). Earlier studies (see for example Refs. [14, 15]) also presented an analysis of data in terms of the KHF, however, in the present work we will limit our comparisons to the results obtained by Pfeiffer *et al.,* as they contained the most current and complete set of data in the fission fragment region known at the time.

The work of Pfeiffer *et al.,* now dates back more than 10 years and since then there have obviously been additional measurements of P_n values to augment the available systematics. While past experiments were concentrated in the fission-fragment region, new radioactive beam facilities have expanded access to a wider variety of nuclei for exploration and determination of P_n values (see for example Refs. [17–20]). In the following, P_n and $T_{1/2}$ values are taken from the most recent version of the Wallet Cards, combined with data from ENSDF [21]. Values with no quoted uncertainty or uncertainties >50% were not considered in the fitting, as they have little influence on the resulting parameters. Another significant advancement since the Pfeiffer work is in the knowledge of Q_β and $Q_{\beta n}$ values for very neutron rich nuclei. Much more precise values are now available due to measurements using Penning traps [22, 23] and storage rings [24]. Q values are taken from the 2011 update to the Atomic Mass evaluation work of Audi *et al.,* [25].

In Fig. 1(a), P_n values in the light fission fragment region with $28 \leq Z \leq 43$ are plotted according to the standard Kratz-Herrmann formula. The improvement in the precision of Q values can be seen by comparing Fig. 1(a) to that of Fig. (2) in Ref. [9]. At the time of the Pfeiffer *et al.,* work, the majority of nuclei considered had appreciable uncertainty on the $Q_{\beta n}/[Q_\beta\text{-C}]$ axis, whereas with the present knowledge of Q values, the uncertainty on the x-axis of Fig. 1(a) has become smaller than the size of the symbols for the majority of the nuclei. The cut-off parameter, C, in the Pfeiffer work was calculated using detailed expressions given in Ref. [16]. Inclusion of this C parameter in the KHF improves the χ^2 of the fit by $\sim$10%. For simplicity, in the following we use C as defined in the original work of Kratz and Herrmann [14] with C=0 for even-even, C=$13/\sqrt{A}$ for odd-even, and C=$26/\sqrt{A}$ for odd-odd nuclei, in units of MeV. The above simple prescription for C is within 5% the values of C used by Pfeiffer *et al.,* and thus, the difference does not have a significant impact on the least-squares fitting procedure. A least-squares fit to the data in Fig. 1(a) gives a reduced χ^2 of 146 and the parameters a=119(42) and b=5.45(48). This is comparable to the Pfeiffer *et al.,* results [9] with reduced χ^2=81, a=106(38) and b=5.51(61). The increase in reduced χ^2 mainly results from the more precisely measured Q values. While there is some overall trend in Fig. 1(a), for any given $Q_{\beta n}/[Q_\beta\text{-C}]$ value, the data span nearly two orders of magnitude. This is obviously reflected in the large reduced χ^2 value and limits the reliability of predictions made using this systematics approach.

TABLE I: Comparison of parameters from a least-squares fit to P_n data. KHF is a fit to P_n data using Eq.(1) and Current is a fit to $P_n/T_{1/2}$ data using Eq. (5).

Ref	Region	Least-squares fit		
		a/c	b/d	χ^2
KHF	$28\leq Z \leq 43$	119(42)	5.45(48)	146
Current	$28\leq Z \leq 43$	0.0097(9)	4.87(7)	35
KHF	$45\leq Z \leq 57$	141(48)	5.08(37)	78
Current	$45\leq Z \leq 57$	0.016(2)	4.55(13)	55
KHF	$Z \leq 25$	45(5)	4.40(40)	280
Current	$Z \leq 25$	0.037(9)	4.11(9)	87

To explore a more compact correlation in P_n values, we start with the basic relations for β-decay quantities. The probability for neutron emission following β decay can be represented schematically as

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

where $S_\beta(E)$ is the β-decay strength function and $f(Z, Q_\beta - E)$ is the Fermi integral. The integral is taken over the β kinetic energy, $(Q_\beta - E)$. The denominator of Eq. (2) is directly related to the half-life with

$$\frac{1}{T_{1/2}} \sim \int_0^{Q_\beta} S_\beta(E) f(Z, Q_\beta - E) dE. \tag{3}$$

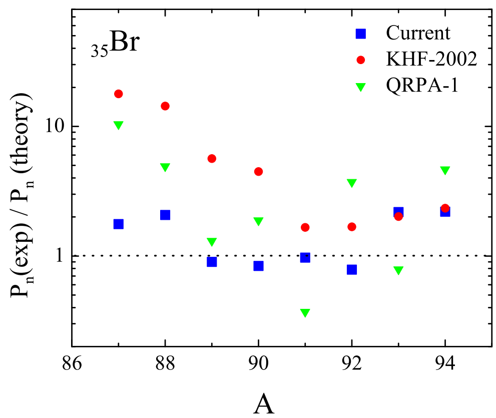

FIG. 2: (Color online) Comparison between experimental P_n values and those predicted by the present work, the KHF [9] and global QPRA calculations [11] for the Bromine isotopes. The comparison is made by considering the ratio of the experimental P_n value to the prediction from the different theories.

From Eqs. (2) and (3), it is clear that there is a natural relation between the P_n value and the half life of the decay; combining these two equations gives

$$\frac{P_n}{T_{1/2}} \sim \int_{S_n}^{Q_\beta} S_\beta(E) f(Z, Q_\beta - E) dE. \quad (4)$$

While papers have touched on the qualitative relationship [9, 26, 27] between $T_{1/2}$ and P_n, surprisingly, a quantitative global study involving these two basic observables has never been performed. As the integral in Eq. (4) is from S_n to Q_β, it seems natural that P_n and $T_{1/2}$ might evolve as a function of the $Q_{\beta n}$ value. We thus investigate the systematics of the ratio $P_n/T_{1/2}$ with

$$\frac{P_n}{T_{1/2}} \sim c Q_{\beta n}^d \quad (5)$$

using a similar parametrization as the KHF. Again, plotted on a log-log scale, one excepts a linear dependence described by the parameters c (intercept) and d (slope). The $P_n/T_{1/2}$ ratio is given in Fig. 1(b) the same nuclei as in Fig. 1(a). Whereas the data plotted in the traditional KHF description shows considerable scatter, plotted instead as $P_n/T_{1/2}$, the data coalesce into a more compact trajectory which can be better described by a single curve. For a given $Q_{\beta n}$ value, the scatter in $P_n/T_{1/2}$ is now reduced to an order of a magnitude or less, allowing for more reliable systematic predictions of P_n. A much improved fit is obtained, with a reduced χ^2 of 35 and the parameters c=0.0097(9) and d=4.87(7). The parameters and reduced χ^2 using the traditional KHF and the current $P_n/T_{1/2}$ ratio are compared in Table I.

The $P_n/T_{1/2}$ ratio provides a simple, yet powerful, method for predicting the systematic behavior of P_n values. In addition, with the data lying on a more compact trajectory, the $P_n/T_{1/2}$ ratio can be useful for identifying and highlighting nuclei that deviate from the overall trend. This concept is illustrated in Fig. 1(b) where two points, with $Q_{\beta n}$ between 1 and 2 MeV, lie substantially above the general trend. Such deviations can point to either incorrectly measured values or provide signatures for new manifestations of nuclear structure. The outliers in Fig. 1(b) correspond to ^{109}Mo and ^{110}Mo, with recently measured [20] P_n values of 1.3(6)% and 2.0(7)%, respectively. The $P_n/T_{1/2}$ systematics predict P_n=0.01-0.03%. Note that in the previous KHF systematics [Fig. 1(a)], the same data do not stand out as being anomalous.

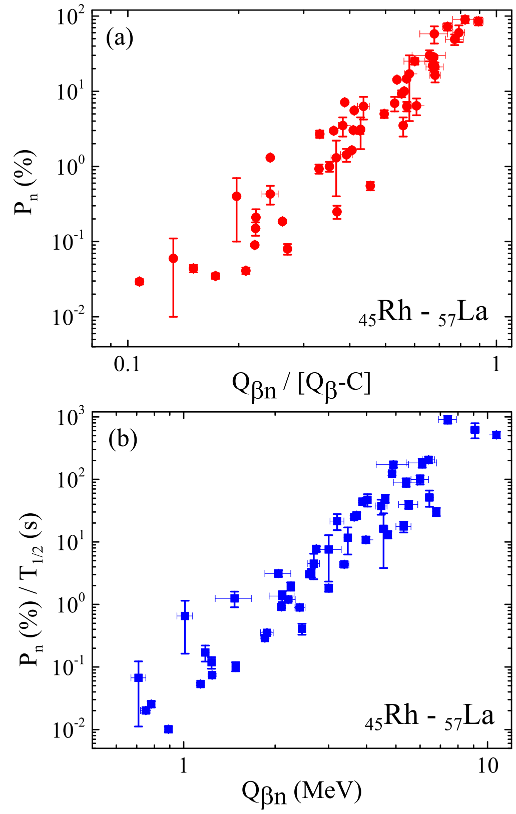

FIG. 3: (Color online) Same as Fig. 1, but for the heavy fission fragment nuclei.

We explore the success of the current approach in Fig. 2 by calculating the P_n values from the c and d parameters given in Table I for the Bromine isotopes. Included are the predictions from the Pfeiffer systematics [9] as well as recent QRPA calculations of Moller *et al.,* [11]. The Bromine isotopes, with high yields in the neutron induced fission of ^{235}U, are well-studied β-delayed neutron emitters and crucial for reactor operation. This chain thus provides a reliable basis for comparison with different systematic and theoretical predictions. With the exception of ^{93}Br, the current predictions using the $P_n/T_{1/2}$ systematics provides the best description of the P_n values

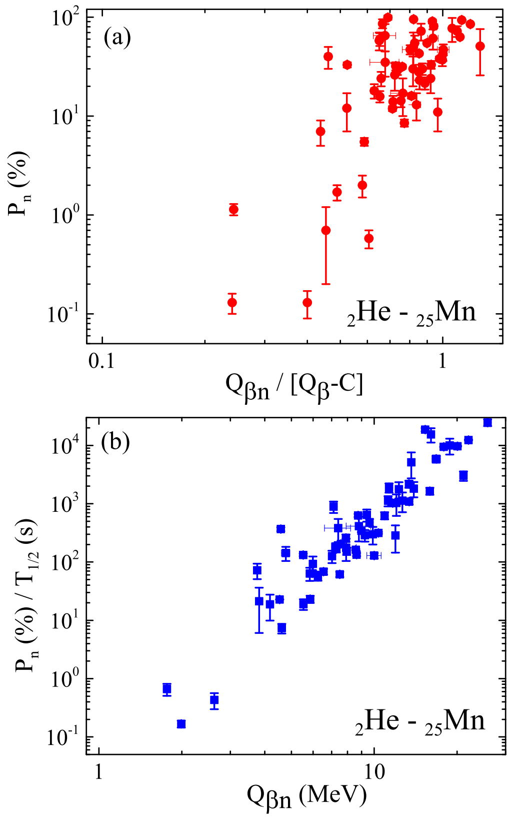

FIG. 4: (Color online) Same as Fig. 1, but for light nuclei with $Z < 26$.

for the Br isotopes. The agreement illustrated in Fig. 2 is overall representative of the level of agreement between the current systematic predictions and experimental P_n values. In general, the $P_n/T_{1/2}$ systematics are within a factor of two or better compared to experiment, although there are a few nuclei which have larger discrepancies.

In Fig. 3(a), the heavy fission fragment region with $45 \leq Z \leq 57$ is plotted in the traditional KHF framework and the parameters of the resulting fit are given in Table I. In Fig. 3(b), the same data are plotted using the ratio $P_n/T_{1/2}$. While there is more scatter in the data for this region compared with the light fission fragments, the $P_n/T_{1/2}$ still provides an improved χ^2 description of the data over the traditional KHF fit. Above Z=57, there is a single nucleus with a measured P_n value; ^{210}Tl with P_n=0.007^{+7}_{-4} %. Using our systematics for the heavy fission fragment region, the b and d parameters predict a P_n of 0.005%, in good agreement with the measured value. We note, however, that the ^{210}Tl value is from an unpublished report [28] and a confirmation of this result as well as additional measurements in this higher mass region would be interesting for exploring the applicability of these systematics across the nuclear chart.

Past investigations have concentrated on the fission fragment regions where sufficient data existed to explore

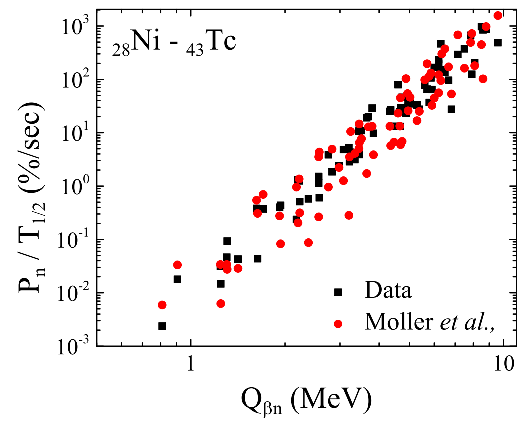

FIG. 5: (Color online) $P_n/T_{1/2}$ plotted as a function of $Q_{\beta n}$ for experimental data (black squares) and the QRPA predictions of Moller *et al.,* [11] (red circles).

systematic trends. One might expect that in lighter nuclei ($Z \leq 25$), where level densities become smaller and shell structure more pronounced, that such systematics would no longer be applicable. Indeed, when considered with the traditional KHF, as given in Fig. 4(a), there is no appreciable trend to the data. A least squares fit to just the P_n systematics gives a very large reduced χ^2 of 280. However, from the standpoint of the $P_n/T_{1/2}$ ratio, even the region of light nuclei exhibits a general systematic behavior, as shown in Fig. 4(b). A least-squares fit to this region gives a much improved reduced χ^2 of 87, suggesting that predictions of P_n values in light nuclei can be made reliable using the $P_n/T_{1/2}$ approach.

There is a simple explanation behind the success of the $P_n/T_{1/2}$ systematics. The P_n value is a ratio of two integrals; the integral of the β-strength function above the neutron separation energy weighted by the Coulomb-distorted phase-space function, divided by the same integral over *all* states. The phase space weighting is very important, as it rises like the fifth power of the energy available for the weak decay. Consequently, it is almost always the lower-lying states in the integrals (near the ground-state or near the neutron separation energy) which dominate the summations. The integral in the numerator starts at the neutron separation energy, usually several MeV above the ground state, so starts in an area of relatively high level density, with states that are usually quite mixed, and rises into an ever-increasing density of states, correlated with a decreasing phase space for the leptons. As a consequence, the strength function is rather smoothly varying and the integral over states is roughly proportional to the size of the energy window where neutron emission is allowed. In contrast, the integral in the denominator is usually dominated by a few transitions close to (or including) the ground state, which are often correlated to the parent β-decaying state, with large matrix elements and large partial widths. Therefore, the denominator is more sensitive to specific nuclear structure effects and fluctuates more rapidly. It is this structure dependence which makes exact calculations of global β-decay rates quite challenging. The suppression of some of these structure dependent matrix elements, by dividing them out in the half-life factor, clearly improves the correlation between $P_n/T_{1/2}$ and $Q_{\beta n}$.

The slope of the $P_n/T_{1/2}$ systematics can provide some insight into the behavior of the strength function in the $Q_{\beta n}$ window. From Eq. (4), if one assumes a constant strength function, then the $P_n/T_{1/2}$ values would simply evolve as the integral of the Fermi function. This integral yields a slope of $\sim$5.3, with only a small dependence on Z. The slope from this very simple approximation is larger than any of the d parameters obtained in the current fits to the data, suggesting a more complicated behavior for the strength function. The Fermi function favors the high-energy β transitions to states just above the neutron separation energy. The fact that the data display a slope less than 5 suggests that the strength function increases with increasing excitation energy, favoring those states with energies closer to the Q_β value. The idea of an energy dependent strength function is certainty not new [29, 30], however, the $P_n/T_{1/2}$ systematics provide an independent confirmation of an increasing strength function for states above the neutron separation energy.

The correlation between P_n and $T_{1/2}$ as given by Eq. (4) suggests that the compact trends observed in Figs. 1, 3 and 4 are a natural manifestation of the underlying physics. We explore this general relationship further using the results of a global QRPA model [11] which incorporates the essential physics of β decay including deformation and first forbidden transitions. At first glance, this model gives substantially different results compared with the systematic predictions, as shown in Fig. 2 using the example of the Bromine isotopes. Here, however, we want not to study specific individual predictions but instead to investigate globally the overall trend of the calculations. Plotted in terms of $P_n/T_{1/2}$, as given in Fig. 5, the overall trend of the QRPA calculations matches very well what is observed in the data. While the results for only the light fission fragments are shown here, a similar correspondence is found for all mass regions.

While the quantity $P_n/T_{1/2}$ provides a more robust way of characterizing the experimental P_n values and can be used for more reliable predictions of P_n values, it does come with the caveat that the $T_{1/2}$ of the parent nucleus needs to be known. This naturally places some restriction on the predictions which can be made using these systematics. Usually, the half-life is one of the first properties of the decay which is determined. With advances in measuring techniques and beam purity, the measurement of half-lives of very neutron rich nuclei can now be performed with only a few hundred implanted ions [19, 31].

In conclusion, we have proposed an improvement to systematic predictions of β-delayed neutron emission probabilities using both the P_n value and the half-life of the decay. We find that the ratio $P_n/T_{1/2}$ has a strong correlation with the allowed Q value for β-delayed neutron emission. Such a correlation holds for all known β delayed neutron emitters, including the very light nuclei.

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