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Transitions between nuclear states represented as steps of a Markov Chain.

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Abstract

In this short document, I will present how transitions between states of a nucleus can be represented as steps of a Markov chain. This expression in a *Markov Matrix* leads to opportunities of using well known matrix formalism, and, when implementing calculations, the existing specialized libraries.

In this document, I will present how to fill a matrix according to transitions probabilities and some examples of using it.

Nuclear levels

As a quantum system, a nucleus can be in a limited number of states of specific spin, parity and excitation energy (defining a “level”). Transition between these levels usually go thru electromagnetic decay (either by emission of a gamma ray or electronic conversion). A specific level does not usually decay to only one other state. The selectivity and probability of decay to another level is governed by their spin, parity, and difference in excitation energy. The probability of decaying from a specific level i to a level j is called the Branching ratio can be noted $P_{i \rightarrow j}$, with the sum of P_i being equal to 1.

Markov Matrix

A Markov (or Stochastic) matrix $[^i, ^j]$ has for specific purpose the notation of transition probability. Therefore, it is natural to use such a matrix to *store* all transitions probabilities between nuclear levels.

With such a vision, the decay path of the nucleus from an excited state to the ground state becomes the steps of a Markov chain [iii, iv]. The expression as a matrix allows simple calculations within codes since many external libraries for general mathematical and scientific libraries already exist to perform operations on matrices [v, vi].

Using the matrix form, one can, for example, compute the average number of gamma ray emitted during a decay from a specific entry point to the ground state. In another way, one can study the Markov matrix to determine which states and transitions are the most important.

Case 1: Average number of gamma emitted in a decay

In the first case study, we look at the β^- decay branch of the well-known ^{152}Eu nucleus. The structure of the daughter nucleus (^{152}Gd) and the branching ratio between the levels are well established [vii, viii] :

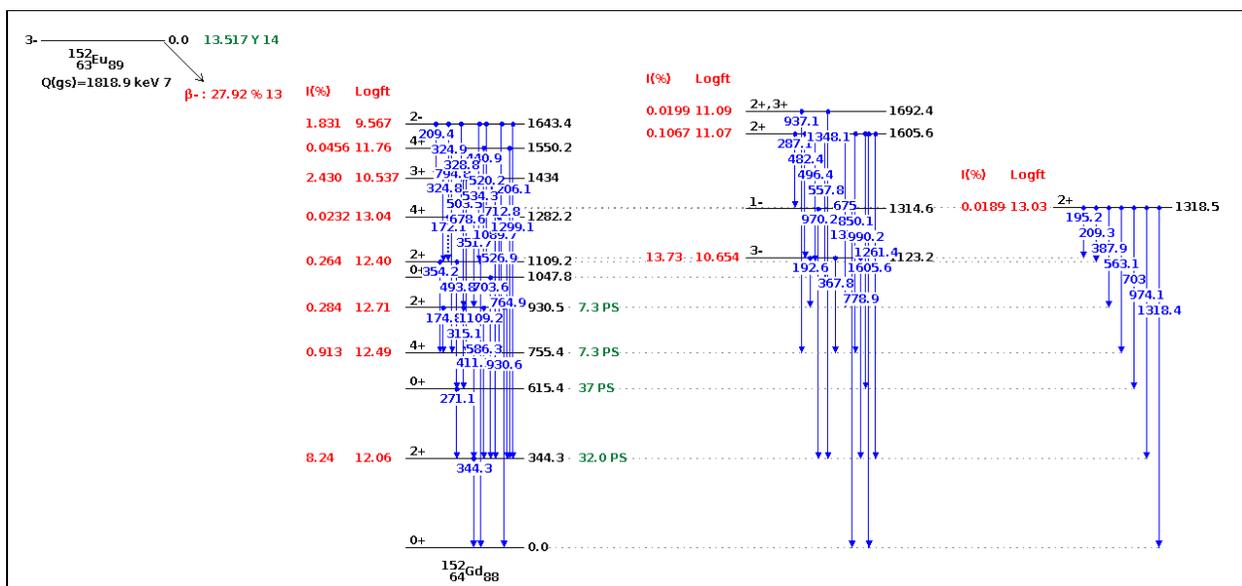


Figure 1: Decay scheme of ^{152}Eu to ^{152}Gd (figure from [viii]).

There are many ways to look at the decay from ^{152}Eu and calculate the average number of transitions between the distribution of entry states and the ground state.

But, reading a computer formatted file, one can fill a matrix with the branching ratios (i.e. probability of transitions from one state to another). Figure 2 shows this matrix.

The next step is to determine the vector of *entry states*, i.e. the starting probabilities of feeding into specific levels when decaying from ^{152}Eu . Figure 3 shows this.

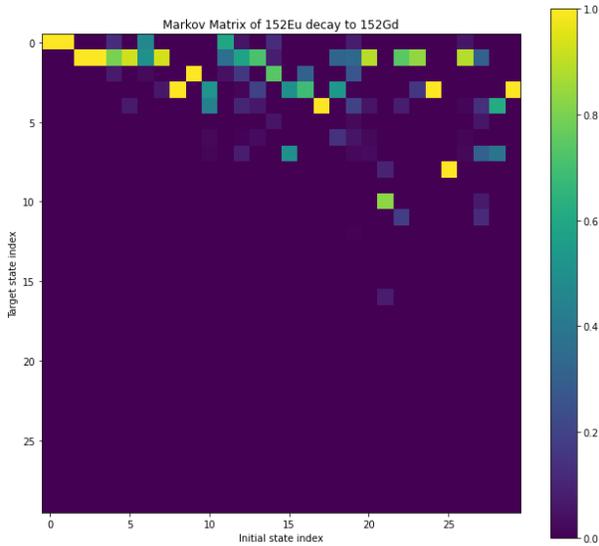


Figure 2: Markov Matrix of ^{152}Gd .

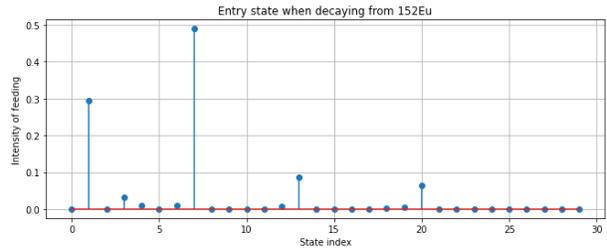


Figure 3: Distribution of entry states when decaying from ^{152}Eu .

One can then perform simple matrix calculations following the example in [ix]. By removing the ground state from the matrix (since it decays only to itself in the convention chosen here), the calculation of $(I - M)^{-1}\mathbf{1}$ (where I is the identity matrix, M the Matrix we built with the transitions probabilities and $\mathbf{1}$ a vector composed of ones) gives the average number of transitions following an entry at a given level. Figure 4 shows the resulting distribution. We notice that the values are close to integer number, but some are in between, because some decay branches can allow a “short cut” that in average gets you from the initial level to the ground state a with one less intermediate state.

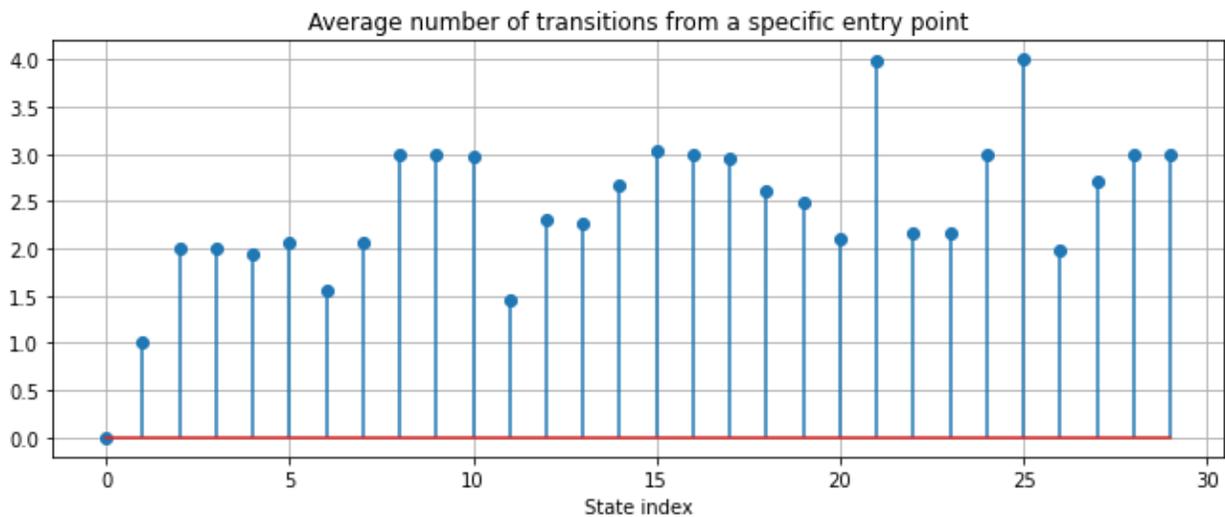


Figure 4: Average number of transitions in ^{152}Gd after an entry at a given level.

Multiplying this result by the entry vector, one obtain the average number of transitions happening for a decay of ^{152}Eu to ^{152}Gd : **1.8**.

Case 2: finding key levels in a nucleus.

In a complex level scheme, it is sometimes hard to find out which level is of importance. It can be useful to identify state that collect and redistribute the “flux” of decay. That can be done easily by just computing $M \cdot \mathbf{1}$ (where M is our transition probability matrix and $\mathbf{1}$ a vector of ones) which return a vector counting the amount of “feeding” each level receives in total from any entry point. This allows the identification of states that are fed more than the others. As expected, the bottom-most levels will have the largest values, with levels above counting less. If a level shows a high value, that singles it out form the others and make it worth scrutiny.

Figure 5 and 6 shows this for ^{238}U . From these figure, one might consider looking at levels number 21 and 23 for example, as they gather more decay intensity than the levels “around” (note that levels of indices close to 23 might have excitation energy and spin far different from those of level 23).

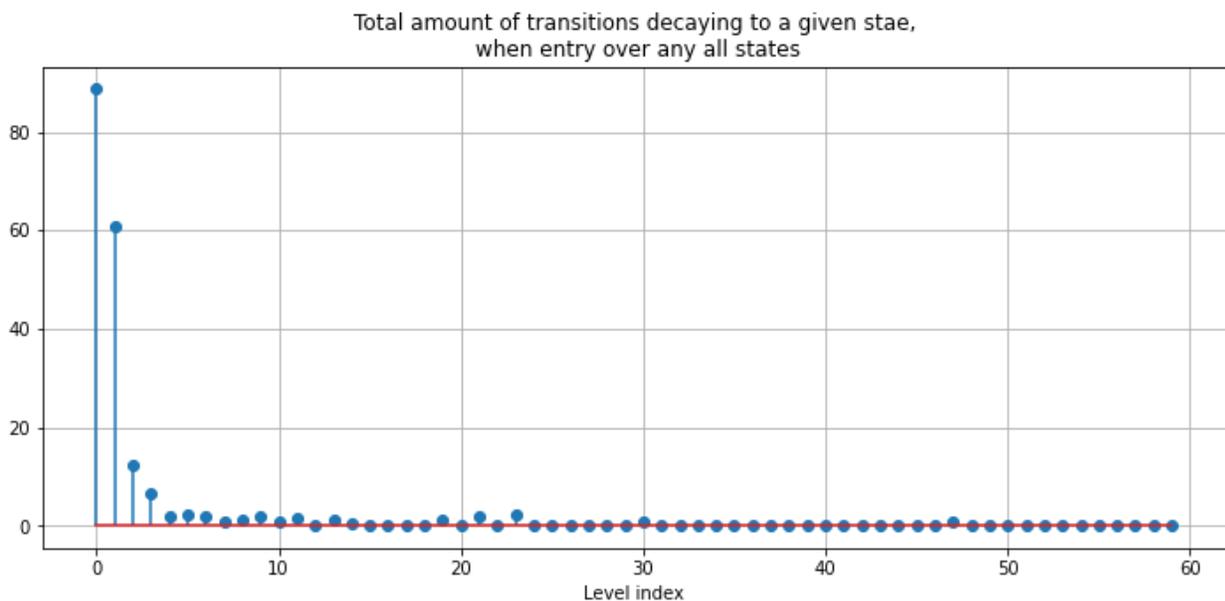


Figure 5: Amount of transitions decaying to a level.

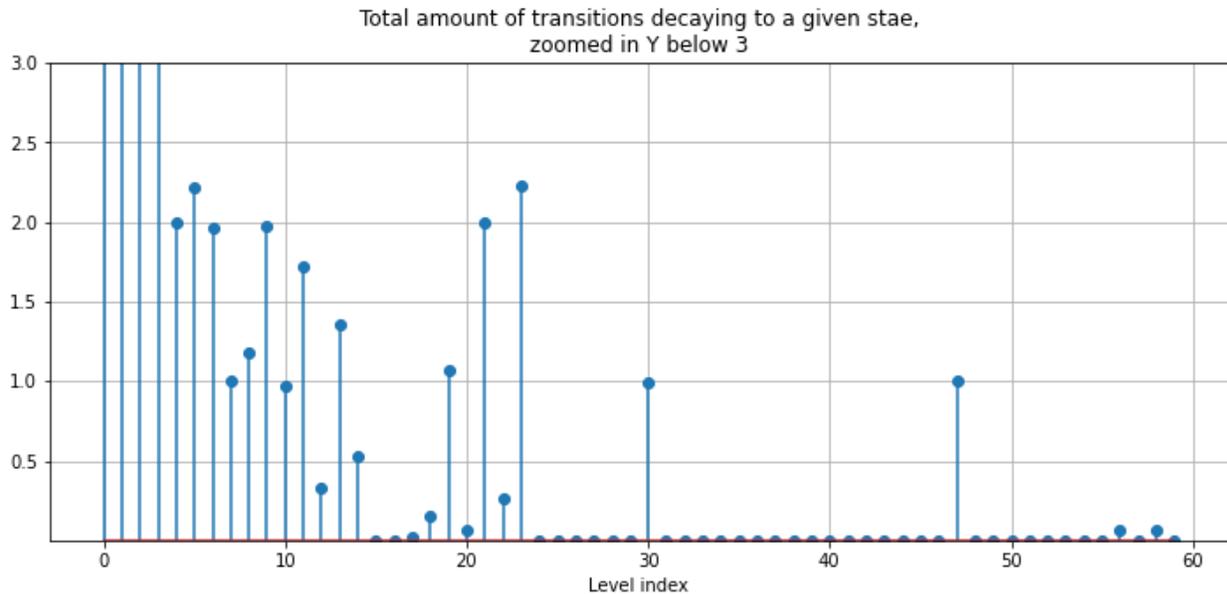


Figure 6: same as figure 5, but zoomed in Y scale.

Conclusion

Using a matrix representation of transitions probabilities between levels in a nucleus is both a nice tool of visualization, but also a great trick to perform calculations. Using dedicated computer library, matrix manipulation can be easy and therefore used in reaction or decay codes to obtain quickly an average number of transitions, for example.

References:

ⁱ <https://deepai.org/machine-learning-glossary-and-terms/stochastic-matrix>

ⁱⁱ https://encyclopediaofmath.org/wiki/Stochastic_matrix

ⁱⁱⁱ <https://towardsdatascience.com/introduction-to-markov-chains-50da3645a50d>

^{iv}

https://www.dartmouth.edu/~chance/teaching_aids/books_articles/probability_book/Chapter11.pdf

^v <https://numpy.org/doc/stable/reference/generated/numpy.matrix.html>

^{vi} https://www.boost.org/doc/libs/1_74_0/libs/numeric/ublas/doc/index.html

^{vii}

[https://www.nndc.bnl.gov/nudat2/getdecaydataset.jsp?nucleus=152GD&dsid=152eu%20bM%20decay%20\(13.517%20y\)](https://www.nndc.bnl.gov/nudat2/getdecaydataset.jsp?nucleus=152GD&dsid=152eu%20bM%20decay%20(13.517%20y))

^{viii} National Nuclear Data Center, information extracted from the NuDat 2 database,
<https://www.nndc.bnl.gov/nudat2/>

^{ix} https://en.wikipedia.org/wiki/Stochastic_matrix#Phase-type_representation