TRAPPER.py: Calculating Transition Probabilities

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January 30, 2017

1 Impetus for this Guide

This document outlines the necessary user inputs needed to calculate transition probabilities using the python3 script TRAPPER.py (TRAnsition Probability Processing/computER).

2 Transition Probabilities

Calculation of the transition probabilities between nuclear states is of importance in nuclear structure physics, as they are used to deduce information about the collectivity of a particular excitation that γ-decays. Equation **??** shows the calculation as a function of quantities that can be measured in laboratory experiments, namely the nuclear lifetime (τ), branching ratio(s)/intensities (BR), conversion coefficients (α), and energy of the γ ray (E_γ).

$$B(\pi\ell; J_i \rightarrow J_f) = \frac{\hbar}{8\pi}\mathcal{F}(\pi\ell)\frac{BR}{\tau(1+\alpha)}\frac{\ell[(2\ell+1)!!]^2}{(\ell+1)}\left(\frac{\hbar c}{E_\gamma}\right)^{2\ell+1} \tag{1}$$

In Equation **??**, $\mathcal{F}(\pi\ell)$ is a measure of the mixing from differing multipolarity γ radiation; For pure E1, E2, or M1 transitions, this factor collapses to unity, where $\mathcal{F}(\pi\ell)$ for mixed E2 & M1 radiation follows the relations in equations **??** & **??**:

$$\mathcal{F}(E2) = \frac{\delta^2}{1+\delta^2} \tag{2}$$

$$\mathcal{F}(M1) = \frac{1}{1+\delta^2} \tag{3}$$

Where δ is the multipole mixing fraction of the particular γ-ray.

This script will take the associated input parameters from the following section and calculate B(E2), B(E1), or B(M1) transition probabilities for each entry. Experimental quantities needed to complete this calculation are the γ-ray energy, the lifetime of the state, the intensity of γ radiation, multipole mixing fraction (if available), and the internal conversion coefficient (if available).

3 Explanation of Input Parameters

Calculation of transition probabilities is automated with the inputs from a comma separated value file (*.csv*). The numerical values needed by the program are explained in the following table and list. There is no limit to the length of the file (TRAPPER.py will calculate *all* transitions automatically). This input file can be made in any cell-editing software (Microsoft Excel, LibreOffice, *etc.*), or manually in a text editor. Values *must* be separated by commas as a delimiter, and according to the template in Table **??**.

line 1	E_γ	δE_γ	I_γ	δ_{I_γ}	$I_{\gamma,tot}$	δ_{mix}	$\delta^+_{\delta_{mix}}$	$\delta^-_{\delta_{mix}}$	τ	δ^+_τ	δ^-_τ	α_K	δ_{α_K}	A	$\pi\ell$	E_{lev}
2	0.888157	0.005	174.8	3.9	369.3	0	0	0	2830	110	110	0.0032	0	162	E2	888.158
⋮	↓	↓	↓	↓	↓	↓	↓	↓	↓	↓	↓	↓	↓	↓	↓	↓

Table 1: Inputs for TRAPPER.py, to be placed in a comma-separated-value worksheet.

Line *1* is ignored by `TRAPPER.py`, and is just a header list for the inputs (for ease of human readability in making the *.csv* file). Lines 2 to X (no limit) are the following values, and must be kept in the same order as listed:

E_γ - the energy of the γ-ray (in MeV)

δE_γ - the uncertainty in the energy of the γ-ray (in keV)

I_γ - the intensity of the specific γ-ray (arbitrary units)

δ_{I_γ} - the uncertainty in the intensity of the γ-ray

$I_{\gamma,tot}$ - the total intensity of *all* γ-decay channels leaving the level

δ_{mix} - the multipole mixing fraction for a γ-ray (0 if no mixing)

$\delta^+_{\delta_{mix}}$ - the upper uncertainty in the multipole mixing fraction

$\delta^-_{\delta_{mix}}$ - the lower uncertainty in the multipole mixing fraction

τ - the lifetime of the *level* in femtoseconds (fs) (**note: this is NOT the half-life**, $\tau \ln(2) = t_{\frac{1}{2}}$)

δ^+_τ - the upper uncertainty in the level lifetime (in fs)

δ^-_τ - the lower uncertainty in the level lifetime (in fs)

α_K - the internal conversion coefficient for a particular γ-ray transition (unitless)

δ_{α_K} - the uncertainty in the internal conversion coefficient

A - the atomic number of the nucleus (used to calculate the Weisskopf estimates)

$\pi\ell$ - the multipolarity of the transition (can be '*E2*', '*E1*', '*M1*', or '*E2(M1)*')

E_{lev} - the level energy of the parent state the γ-ray is decaying from (not actually used in the calculation)

One of the key entries is the column $\pi\ell$, as this flag determines which B($\pi\ell$) calculation will be output. 'E2' will tell the calculator to output the B(E2) calculation and error (in W.u.), 'E1' will have `TRAPPER.py` output the B(E1) (in mW.u.), 'M1' outputs the B(M1) (in μ_N^2), while 'E2(M1)' will output the B(E2) calculation assuming there is a mixed-multipole transition. This calculation will only succeed if δ_{mix} is nonzero and is reported in Weisskopf units, as if it were a mixed strength E2!!!

A final note on input parameters: if the absolute intensity is not known, then the branching ratio can be input in place of I_γ, as long as $I_{\gamma,tot}$ is '1'. Ideally, one runs `TRAPPER.py` in the same directory as the *.csv* file, but can reference a file in another directory by pointing (relative to the present working directory) to the file.

4 Script Execution

`TRAPPER.py` requires two standard python3 libraries to successfully run: `numpy` and `scipy`, the former being used for data-input convenience, and the latter for physical constant precision.

Running this script is simple; one only needs to execute the script in one's terminal via:

```
$ python3 TRAPPER.py
```

Assuming the user has the correct libraries install to his/her system, a prompt will appear in your terminal to have the user point to the input and desired output files. Simply enter the path when prompted, and the calculation output will appear in your terminal. In the case of an error, check your current bash configuration (or default python3/terminal environment). On some systems, you may need to invoke:

```
$ python3.X TRAPPER.py
```

depending on your current version of python3.X.

5 Method of Output for B($\pi\ell$) Values

For quick reference, `TRAPPER.py` will output the calculations to both the local terminal as well as to an output file, (to the location the user specifies) with similar outputs to the terminal. This output file is LaTeX-friendly, in that a table generated via this method will be *ready* to cut and paste into an existing TEX document. An example of the table of outputs generated is given in Table **??**; the user is encouraged to manually tweak any formatting errors that could arise (though ideally not encountered). The author assumes the user is capable of editing LaTeXtables in a text editor to add various stylings such as horizontal lines, the removal of columns/entries altogether, as well as a conversion of the table into the `longtable` table environment, but the default setting (to potentially be changed later) outputs the level energy, the γ-ray energy, the intensity of the transition, the nuclear lifetime, the multipolarity of the transition and any associated mixing present (only relevant for E2/M1 transitions), and the final calculation of B($\pi\ell$) with corresponding units.

Rounding of calculations do not occur until the very end, and are rounded to 2 decimal point precision.

On the subject of error propagation: For quantities with a symmetric uncertainty associated with the quantity (E_γ, I_γ, α), error propagation occurs as expected, added in quadrature (the author assumes the reader is familiar with standard error propagation techniques via derivitaves of Equation **??**), while asymmetric quantities (τ) are propagated by subtracting the *nominal* values from the largest/smallest value for B, and are then incorporated into the standard error propagation. This justification is made in *R. Barlow, PHYSTAT2003, SLAC. Stanford, California, September 8-11, (2003).*

E_{lev} (keV)	E_γ (keV)	I_γ	τ (fs)	$\pi\ell$	δ	B($\pi\ell$) (W.u.)
888.16	888.16 (3)	174.8 (39)	$2830^{+110.0}_{-110.0}$	E2	$0.0\ ^{+0.0}_{0.0}$	$4.69\ ^{+4.49}_{-4.88}$
888.16	807.5 (2)	184.5 (48)	$2830^{+110.0}_{-110.0}$	E2	$0.0\ ^{+0.0}_{0.0}$	$7.97\ ^{+7.63}_{-8.29}$
888.16	622.49 (3)	3.7 (1)	$2830^{+110.0}_{-110.0}$	E2	$0.0\ ^{+0.0}_{0.0}$	$0.59\ ^{+0.59}_{-0.61}$
1148.23	260.07 (8)	129.0 (20)	$300000^{+600.0}_{-600.0}$	E1	$0.0\ ^{+0.0}_{0.0}$	$0.05\ ^{+0.05}_{-0.05}$
1148.23	185.29 (1)	26.7 (11)	$300000^{+600.0}_{-600.0}$	E1	$0.0\ ^{+0.0}_{0.0}$	$0.03\ ^{+0.03}_{-0.03}$
1275.77	1275.81 (18)	30.3 (8)	$29^{+5.0}_{-5.0}$	E1	$0.0\ ^{+0.0}_{0.0}$	$2.31\ ^{+1.81}_{-2.79}$
1275.77	1195.09 (7)	41.3 (32)	$29^{+5.0}_{-5.0}$	E1	$0.0\ ^{+0.0}_{0.0}$	$3.82\ ^{+3.02}_{-4.62}$
1357.92	1277.27 (11)	64.3 (12)	$214^{+0.0}_{0.0}$	E1	$0.0\ ^{+0.0}_{0.0}$	$0.43\ ^{+0.43}_{-0.43}$
1357.92	1092.26 (6)	46.6 (30)	$214^{+0.0}_{0.0}$	E1	$0.0\ ^{+0.0}_{0.0}$	$0.49\ ^{+0.49}_{-0.49}$
1485.67	1219.98 (34)	26.6 (8)	$2910^{+0.0}_{0.0}$	E1	$0.0\ ^{+0.0}_{0.0}$	$0.04\ ^{+0.04}_{-0.04}$
1485.67	937.14 (7)	12.0 (8)	$2910^{+0.0}_{0.0}$	E1	$0.0\ ^{+0.0}_{0.0}$	$0.04\ ^{+0.04}_{-0.04}$
1485.67	424.68 (4)	0.5 (0)	$2910^{+0.0}_{0.0}$	E1	$0.0\ ^{+0.0}_{0.0}$	$0.02\ ^{+0.02}_{-0.02}$
1485.67	302.91 (2)	0.4 (0)	$2910^{+0.0}_{0.0}$	E1	$0.0\ ^{+0.0}_{0.0}$	$0.04\ ^{+0.04}_{-0.04}$
1485.67	275.58 (4)	0.8 (0)	$2910^{+0.0}_{0.0}$	E1	$0.0\ ^{+0.0}_{0.0}$	$0.1\ ^{+0.1}_{-0.1}$
1485.67	188.66 (3)	0.2 (0)	$2910^{+0.0}_{0.0}$	E2	$0.0\ ^{+0.0}_{0.0}$	$106.6\ ^{+33.38}_{-118.82}$
1485.67	161.21 (5)	0.1 (0)	$2910^{+0.0}_{0.0}$	M1	$0.0\ ^{+0.0}_{0.0}$	$0.0\ ^{+0.0}_{0.0}$
1485.67	95.16 (1)	0.4 (0)	$2910^{+0.0}_{0.0}$	E2(M1)	$0.0\ ^{+0.0}_{0.0}$	$7500.76\ ^{+-103633.57}_{-104641.49}$
1518.42	1252.74 (29)	26.0 (20)	$193^{+0.0}_{0.0}$	E1	$0.0\ ^{+0.0}_{0.0}$	$0.61\ ^{+0.56}_{-0.61}$
1518.42	969.91 (6)	10.9 (4)	$193^{+0.0}_{0.0}$	E1	$0.0\ ^{+0.0}_{0.0}$	$0.55\ ^{+0.55}_{-0.55}$
1518.42	457.48 (40)	0.0 (0)	$193^{+0.0}_{0.0}$	E1	$0.0\ ^{+0.0}_{0.0}$	$0.02\ ^{+0.02}_{-0.01}$
1518.42	160.49 (4)	0.2 (0)	$193^{+0.0}_{0.0}$	E2	$0.0\ ^{+0.0}_{0.0}$	$3265.29\ ^{+-38385.6}_{-38894.47}$
1862.67	714.44 (5)	6.1 (5)	$2860^{+0.0}_{0.0}$	E2	$0.0\ ^{+0.0}_{0.0}$	$6.95\ ^{+6.54}_{-6.96}$
1862.67	652.58 (3)	2.9 (0)	$2860^{+0.0}_{0.0}$	E2	$0.0\ ^{+0.0}_{0.0}$	$5.26\ ^{+5.14}_{-5.26}$
1862.67	377.02 (5)	0.2 (0)	$2860^{+0.0}_{0.0}$	E2(M1)	$0.0\ ^{+0.0}_{0.0}$	$6.19\ ^{+5.77}_{-6.2}$
1862.67	327.01 (1)	13.9 (2)	$2860^{+0.0}_{0.0}$	E1	$0.0\ ^{+0.0}_{0.0}$	$1.78\ ^{+1.78}_{-1.78}$
1862.67	228.26 (1)	1.4 (0)	$2860^{+0.0}_{0.0}$	E1	$0.0\ ^{+0.0}_{0.0}$	$0.54\ ^{+0.54}_{-0.54}$
1910.42	1022.28 (11)	8.3 (5)	$305^{+0.0}_{0.0}$	E1	$0.0\ ^{+0.0}_{0.0}$	$0.34\ ^{+0.34}_{-0.34}$
1910.42	947.48 (8)	8.9 (3)	$305^{+0.0}_{0.0}$	E1	$0.0\ ^{+0.0}_{0.0}$	$0.46\ ^{+0.46}_{-0.46}$
1910.42	849.44 (7)	7.1 (2)	$305^{+0.0}_{0.0}$	E1	$0.0\ ^{+0.0}_{0.0}$	$0.51\ ^{+0.51}_{-0.51}$
1910.42	552.49 (21)	0.1 (0)	$305^{+0.0}_{0.0}$	E2(M1)	$0.0\ ^{+0.0}_{0.0}$	$3.62\ ^{+2.88}_{-3.66}$
1862.67	714.44 (5)	6.1 (5)	$1580^{+0.0}_{0.0}$	E2	$0.0\ ^{+0.0}_{0.0}$	$12.58\ ^{+11.42}_{-12.61}$
1862.67	652.58 (3)	2.9 (0)	$1580^{+0.0}_{0.0}$	E2	$0.0\ ^{+0.0}_{0.0}$	$9.51\ ^{+9.28}_{-9.51}$
1862.67	377.02 (5)	0.2 (0)	$1580^{+0.0}_{0.0}$	E2(M1)	$0.0\ ^{+0.0}_{0.0}$	$11.2\ ^{+10.41}_{-11.21}$
1862.67	327.01 (1)	13.9 (2)	$1580^{+0.0}_{0.0}$	E1	$0.0\ ^{+0.0}_{0.0}$	$3.22\ ^{+3.18}_{-3.22}$
1862.67	228.26 (1)	1.4 (0)	$1580^{+0.0}_{0.0}$	E1	$0.0\ ^{+0.0}_{0.0}$	$0.97\ ^{+0.97}_{-0.97}$
1910.42	1022.28 (11)	8.3 (5)	$253^{+0.0}_{0.0}$	E1	$0.0\ ^{+0.0}_{0.0}$	$0.41\ ^{+0.41}_{-0.41}$
1910.42	947.48 (8)	8.9 (3)	$253^{+0.0}_{0.0}$	E1	$0.0\ ^{+0.0}_{0.0}$	$0.56\ ^{+0.56}_{-0.56}$
1910.42	849.44 (7)	7.1 (2)	$253^{+0.0}_{0.0}$	E1	$0.0\ ^{+0.0}_{0.0}$	$0.62\ ^{+0.62}_{-0.62}$
1910.42	552.49 (21)	0.1 (0)	$253^{+0.0}_{0.0}$	E2(M1)	$0.0\ ^{+0.0}_{0.0}$	$4.36\ ^{+3.44}_{-4.41}$

Table 2: REMEMBER TO CHANGE TABLE CAPTION AND REFERENCE TAG HERE!