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Python Graphical User Interface for Product Operator Formalism of Spin-1/2 for Nuclear Magnetic Resonance

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Purpose

This program is designed to handle the product operator formalism of spin-1/2 nuclei for Nuclear Magnetic Resonance (NMR) using Python Graphical User Interface (GUI). The GUI is designed with high flexibility. The program will be helpful for educational use, for example, showing how to calculate product operators and explaining how pulse sequence components, such as Hahn-echo, INEPT etc., work.

Requirements

This program uses a module to calculate product operators on Python. Please get the module from https://github.com/ohgo1977/ProductOperator_Python . Please see the requirement to run the module. The GUI was built with Tkinter. This program was tested under Python 3.8.5 and 3.10.11 with Windows 10 PCs.

How to Use Program

How to Launch GUI window

There are several ways to launch the GUI window for the program. One way is 1) Open PO_GUI.py in IDLE, and 2) Run > Run Module. Then, the GUI window is launched.

From the terminal, type in

```
> python PO_GUI.py
```

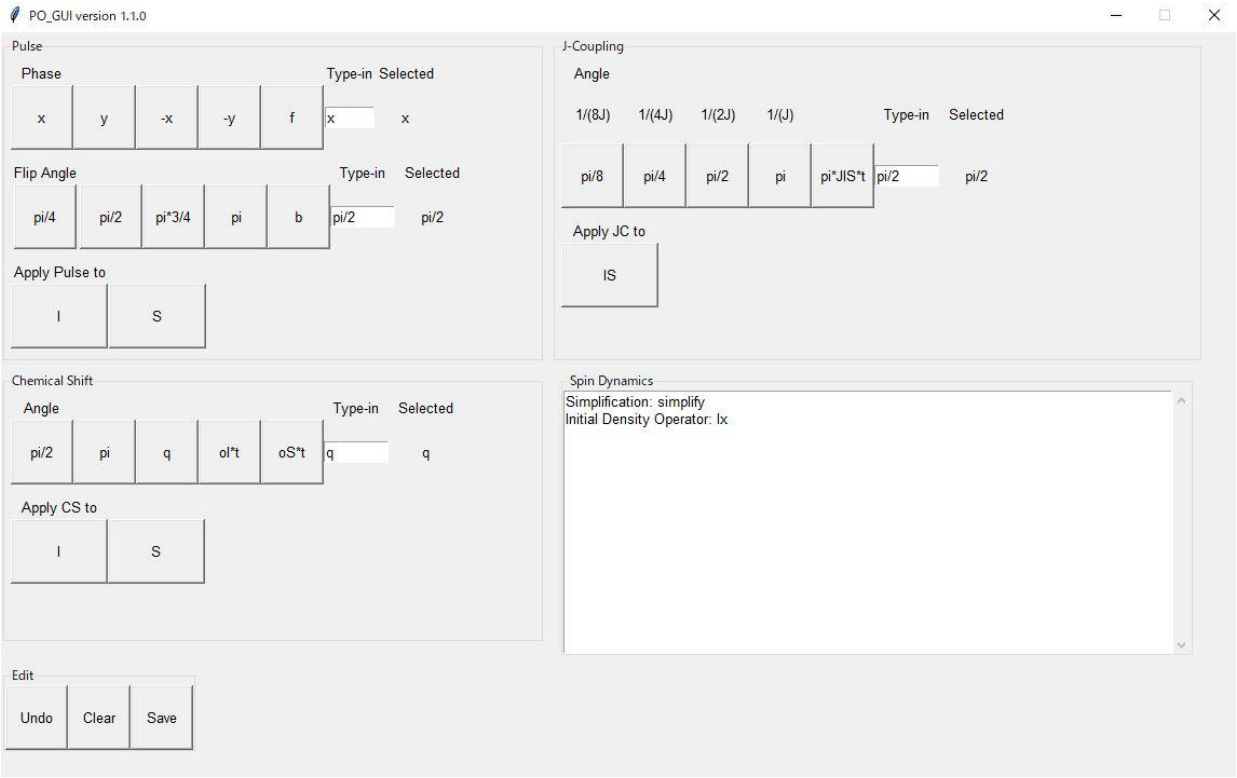
Initial Setup

Three questions will appear in the terminal window for the initial setup.

```
Enter Method for Simplification (simplify, TR8, fu, Default: simplify):
Enter Spin Labels Separated by Commas (Default: I,S):
Enter Initial Density Operator (Default: Iz + Sz):
```

The first question is to select a method used for the simplification process (please see the manual of PO.py for the details). If you use the default method, simplify, hit the Enter key. The second question is the labels of spins you like to use. For example, if you like to create a 3-spin systems with [I1, I2, I3], input I1,I2,I3. The default value is I,S for the I-S spin system. The third question is the initial density operator. You can use arbitrary coefficients with the spin operators, e.g., ai*Ix*cos(qi). The default value is a sum of z-operators generated automatically from the spin labels (e.g., Iz + Sz for I-S spin system).

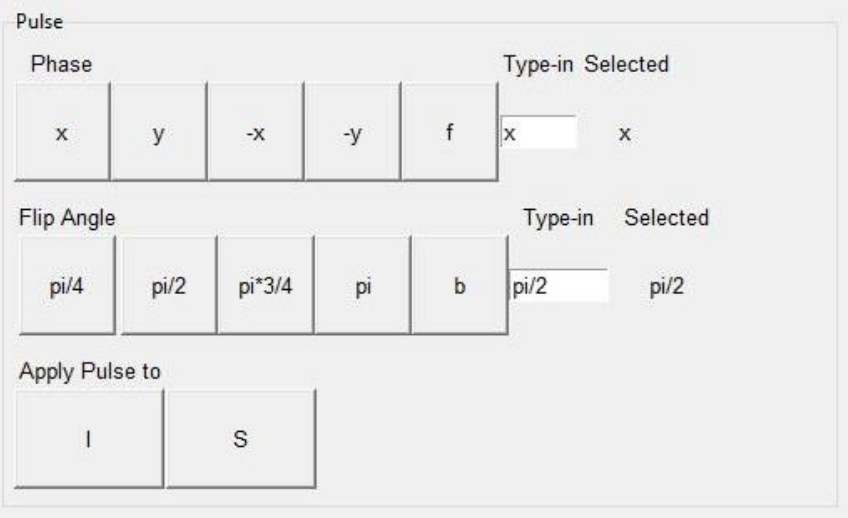
Then, the GUI window appears.



The figure above is the case of the I-S spin system, Ix as an initial density operator, and simplify as the simplification method.

Pulse Frame

The GUI for the pulse is shown below.



1st row: Phase

You can select a phase from the quadrature phases, a phase ‘f’, or arbitrary phase that can be typed in.

2nd row: Flip Angle

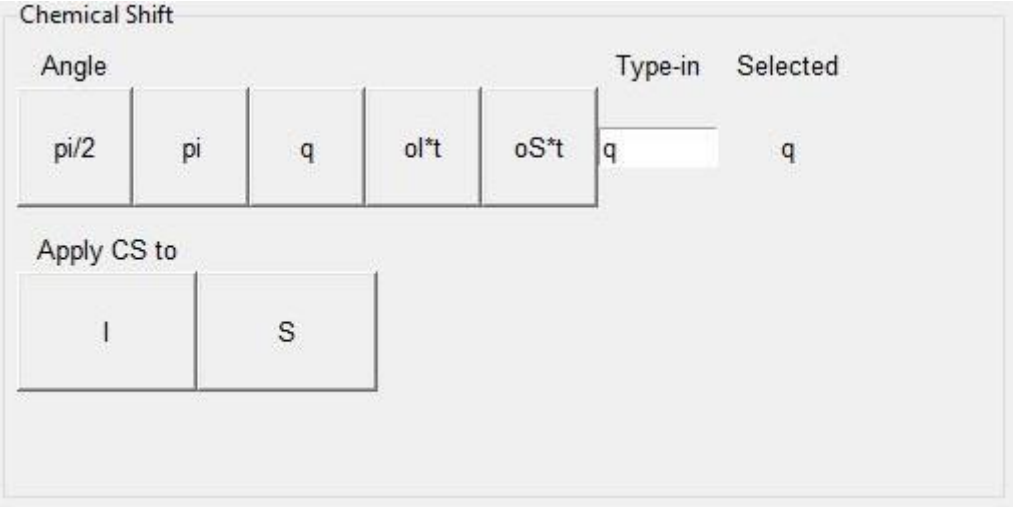
You can select a flip angle from pi/4, pi/2, pi*3/4, pi, an angle ‘b’, or arbitrary angle that can be typed in.

3rd row: Spin Type

You can apply a pulse with the selected phase and flip angle to one of the spins. The number and labels of the buttons will be automatically generated from the spin labels you entered at the initial setup.

Chemical Shift Frame

The GUI for the chemical shift is shown below.



1st row row: Angle

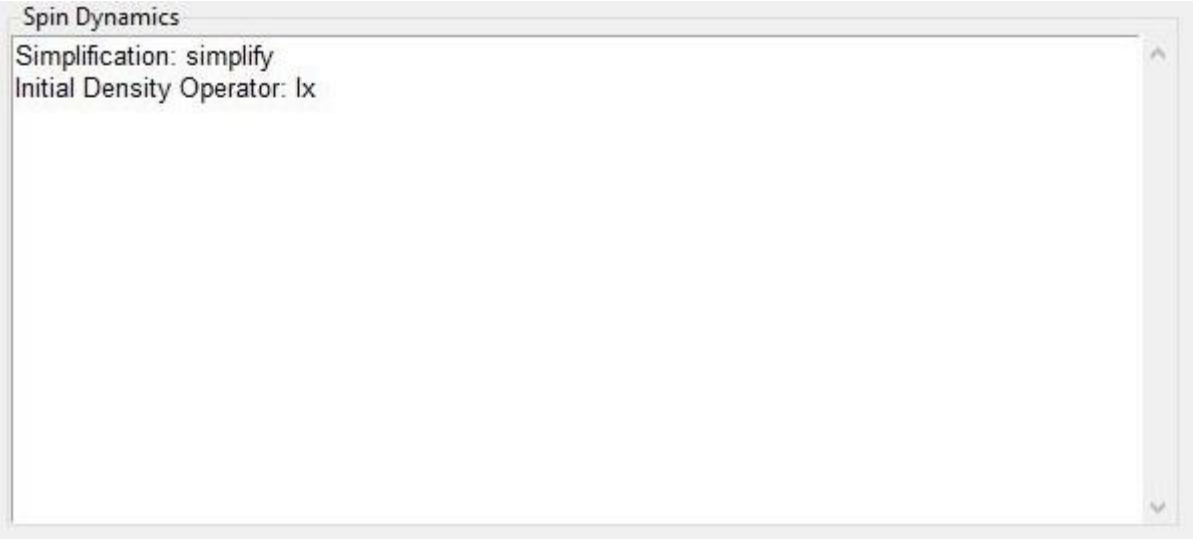
You can select an angle of the chemical shift evolution from pi/2, pi, ‘q’, ‘oI*t’, ‘oS*t’, or arbitrary angle that can be typed in. Note that ‘I’ and ‘S’ in ‘oI’ and ‘oS’ are automatically labeled from the spin labels.

2nd row: Spin Type

You can select a spin type for the chemical shift evolution with the angle selected. Same as the pulse frame, the buttons are automatically generated based on the the spin labels.

Spin Dynamics Frame

The result of the calculation is shown in the text frame. A slide will appear once the results don't fix in the frame.



Edit Frame

The GUI for editing is shown below.

'Undo' Button

You can undo the process by this button.

'Clear' Button

You can start the process from the initial state you type in.

'Save' Button

You can save the text in the text box to a text file. A dialog will appear for saving.

Examples

Hahn-echo in 1-spin system

In this example, the initial density operator Iz becomes Ix by a $\pi/2_y$ pulse followed by the chemical shift evolution. Then, a π_x pulse is applied. After the second chemical shift evolution, the density operator becomes Ix again, meaning that the chemical shift is refocused.

```
Simplification: simplify
Initial Density Operator: Iz

Pulse: I  90y
   Ix

CS: I q
   Ix*(cos(q)) + Iy*(sin(q))

Pulse: I 180x
   Ix*(cos(q)) + Iy*(-sin(q))

CS: I q
   Ix
```

Spin-echo in 2-spin system for J-decoupling

In this example, the magnetization Ix evolves under the chemical shift and J-coupling. Then a π-pulse is applied to the S-spin. After the second period of chemical shift and J-coupling, only the chemical shift evolves with the angle of 2*oI*t.

```
Simplification: simplify
Initial Density Operator: Ix

CS: I oI*t
   Ix*(cos(oI*t)) + Iy*(sin(oI*t))

JC: IS pi*JIS*t
   Ix*(cos(oI*t)*cos(pi*JIS*t)) + 2IxSz*(-sin(oI*t)*sin(pi*JIS*t)) +
Iy*(sin(oI*t)*cos(pi*JIS*t)) + 2IySz*(sin(pi*JIS*t)*cos(oI*t))
```

```
Pulse: S 180x
   Ix*(cos(oI*t)*cos(pi*JIS*t)) + 2IxSz*(sin(oI*t)*sin(pi*JIS*t)) +
Iy*(sin(oI*t)*cos(pi*JIS*t)) + 2IySz*(-sin(pi*JIS*t)*cos(oI*t))

CS: I oI*t
   Ix*(cos(2*oI*t)*cos(pi*JIS*t)) + 2IxSz*(cos(t*(pi*JIS - 2*oI))/2 -
cos(t*(pi*JIS + 2*oI))/2) + Iy*(-sin(t*(pi*JIS - 2*oI))/2 + sin(t*(pi*JIS + 2*oI))/2)
+ 2IySz*(-sin(pi*JIS*t)*cos(2*oI*t))

JC: IS pi*JIS*t
   Ix*(cos(2*oI*t)) + Iy*(sin(2*oI*t))
```

References

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Keeler, J., *Understanding NMR Spectroscopy*, 1st Edition, Wiley, **2005**.

Hassan, J., Nabulsi, A. A., *A New Graphical User Interface for Teaching NMR*, *Am. J. Edu. Res.*, **2014**, *2*, 240-244.

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