SpinDrops Tutorial

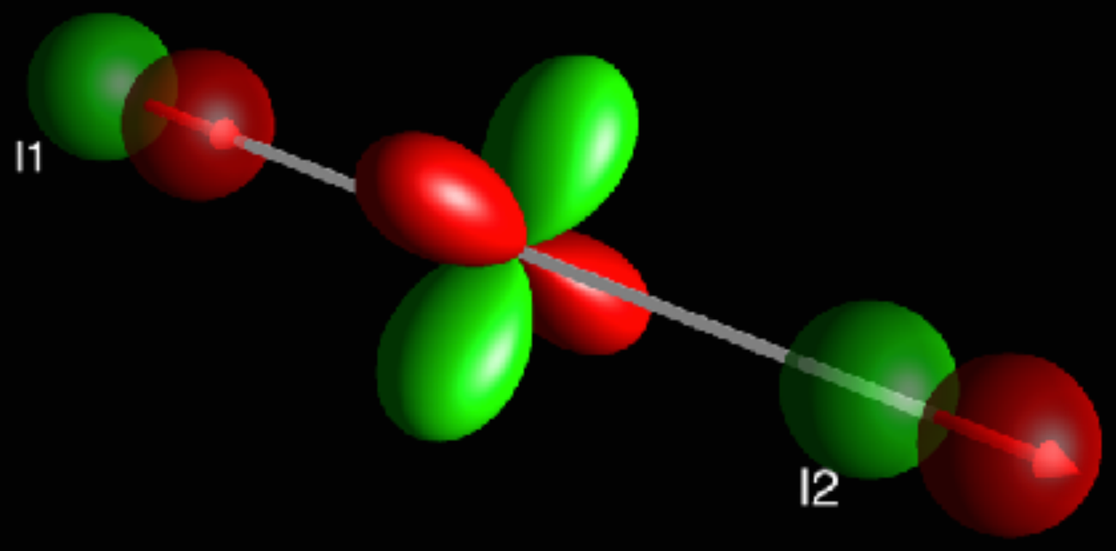
Introduction

SpinDrops provides an interactive approach to visualize the rich dynamics of spin systems. The app is based on the so-called DROPS representation (A. Garon et al., 2015), which provides a general approach for the visualization of arbitrary spin operators.

The interactivity of *SpinDrops* allows you to explore the app (and the world of spins) simply by trying different options and parameters. The following tutorial and the material in the *Help* menu provide useful background information to become familiar with the handling of the app and with the DROPS representation.

In the *Help* menu, you will also find a number of *Challenges* that you may want to tackle and try to solve!

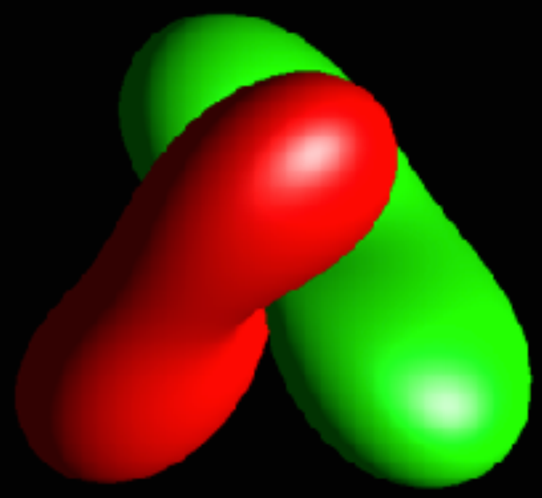
PDF files of the *Help* menu can also be downloaded at *http://www.glasersystems.de/manuals.*



Why use the app?

Here is a top 5 list of some of the best reasons why using the app may be worthwhile:

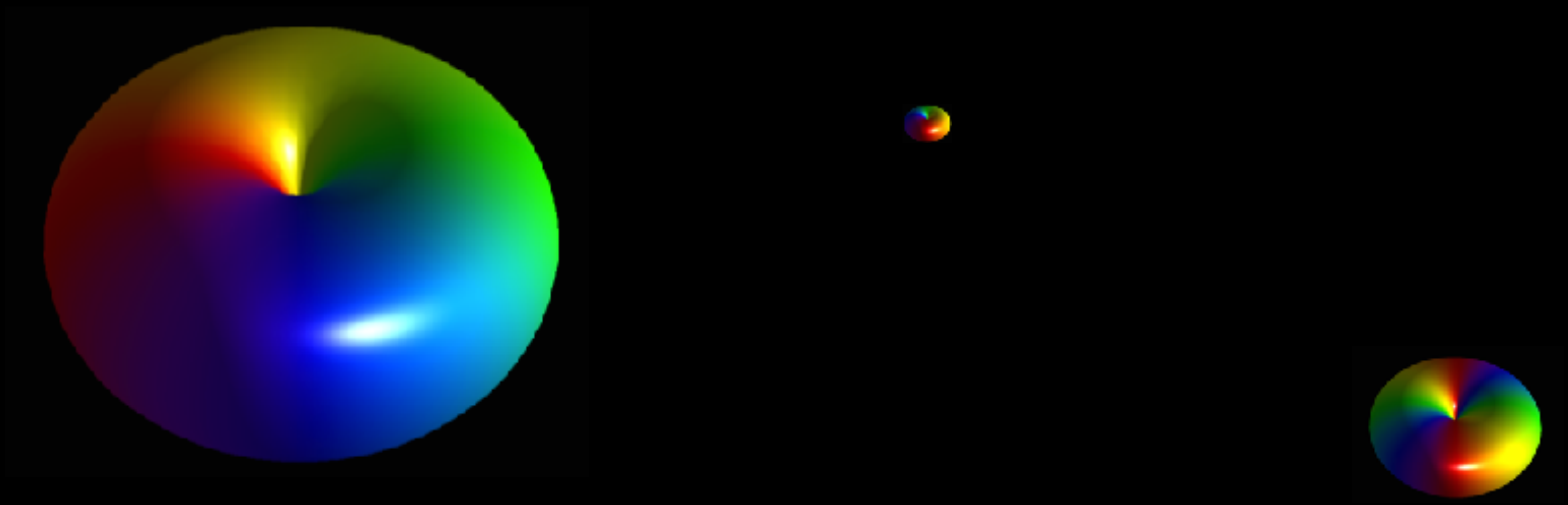
(1) Have fun with spin dynamics.
(2) Actually *see* what is going on in an experiment.
(3) Understand the properties of spin operators.
(4) Develop intuition about the effects of pulse sequences.
(5) Become familiar with standard experimental building blocks, invent and test novel pulse sequences.



What will I learn?

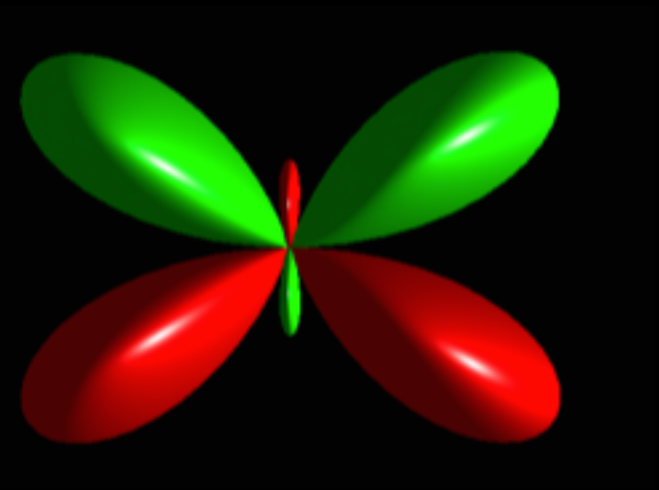
Top 5 concepts that can be learned by working and playing with *SpinDrops*:

(1) Effects of non-selective and selective rotations on spin operators.
(2) Effects of frequency offsets and spin-spin couplings.
(3) Effects of various experimental building blocks to manipulate the state of a spin system.
(4) Product operators (antiphase operators, multiple-quantum coherence, coherence order).
(5) Principles of polarization and coherence transfer.



Limitations of the Cartesian product operator formalism

In version 1.2 of *SpinDrops*, simulations are based on the standard Cartesian product operator formalism. This elegant formalism provides simple analytical expressions to calculate the dynamics of coupled spins. However, it also has some limitations:



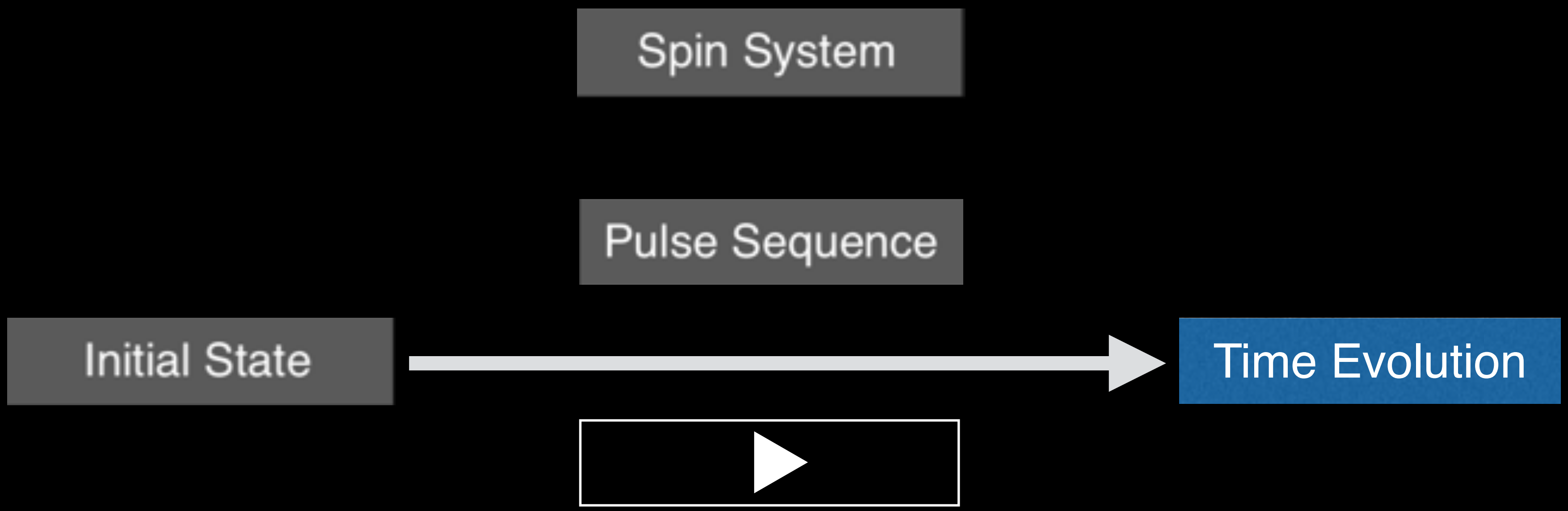
- Ideal pulses are assumed, i.e. the effects of frequency offsets and couplings are not taken into account during the pulses.

- During delays, the weak coupling limit is assumed. For heteronuclear spins, this is always an excellent approximation. However, the simulations of homonuclear spin systems is not exact if strong coupling effects play a role (i.e. if the offset-difference of two spins is on the same order of magnitude as the *J* coupling between them). This is not a problem as long as you are aware of this limitation. In fact, it allows you to see and study the effects of simultaneous offset and weak coupling evolution on a comparable time-scale, which would not be possible otherwise. Although strong coupling effects are neglected during delays, they are fully taken into account in the simulation of spin dynamics of two coupled spins under isotropic mixing conditions (in TOCSY and TACSY experiments).

How to Use the SpinDrops App

The app can be used in many different ways and you are encouraged to explore these possibilities in your own way. A typical approach to see the spin dynamics created by a given pulse sequence involves the following steps:

- Select a *spin system* and its parameters (offset frequencies and coupling constants).
- Choose the *initial state* of the spin system (e.g. z magnetization of spin I_1).
- Pick a *pulse sequence* (e.g. a 90° pulse followed by a delay).
- *Run* the pulse sequence by touching the play icon (▶) and see the resulting time evolution in the DROPS display.



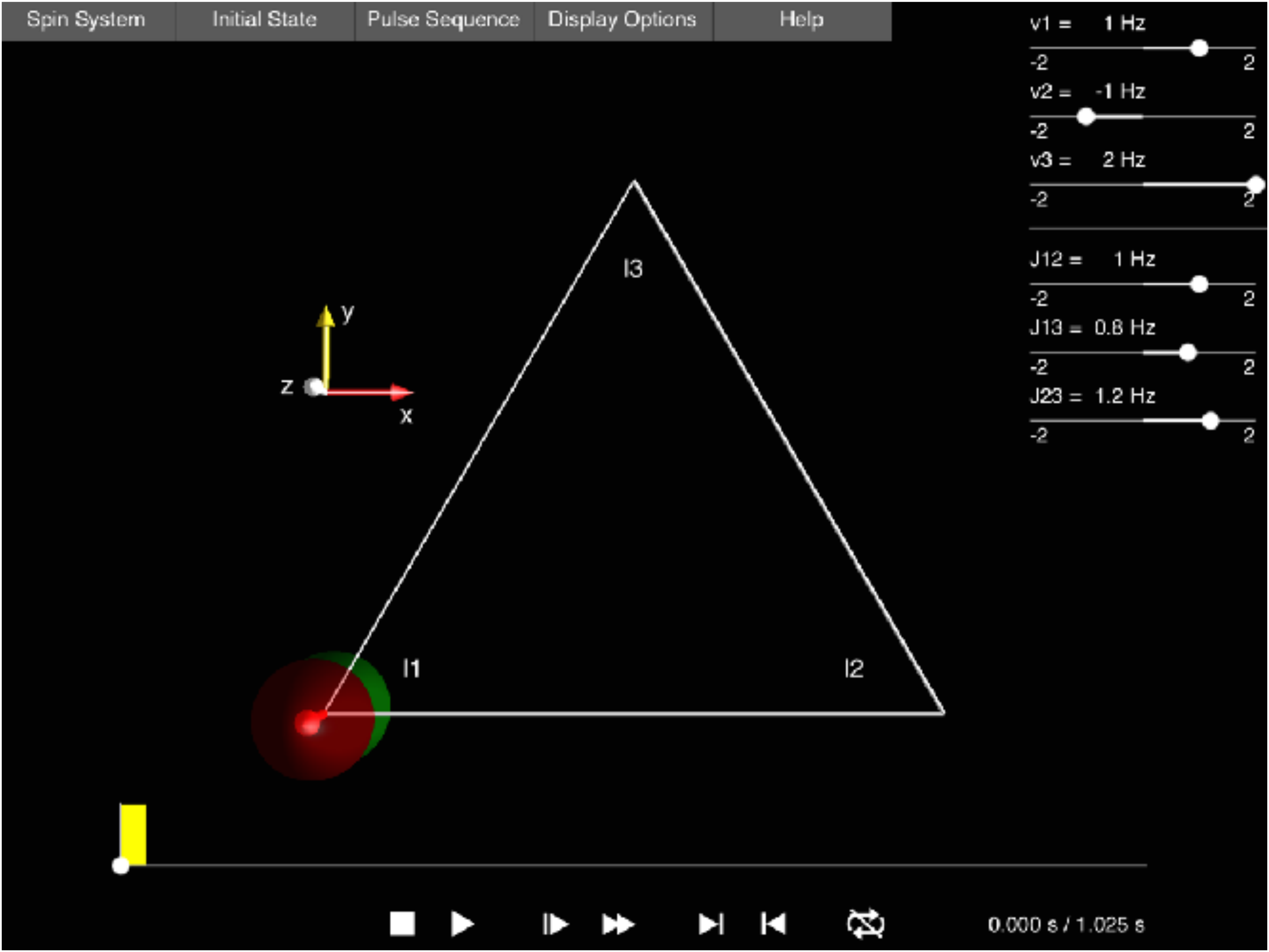
The Start Screen

Menu Panel

DROPS Display

Pulse Sequence

Control Panel



v1 = 1 Hz

v2 = -1 Hz

v3 = 2 Hz

J12 = 1 Hz

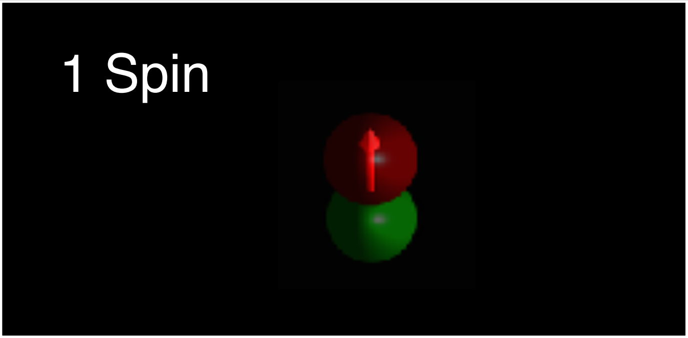
J13 = 0.8 Hz

J23 = 1.2 Hz

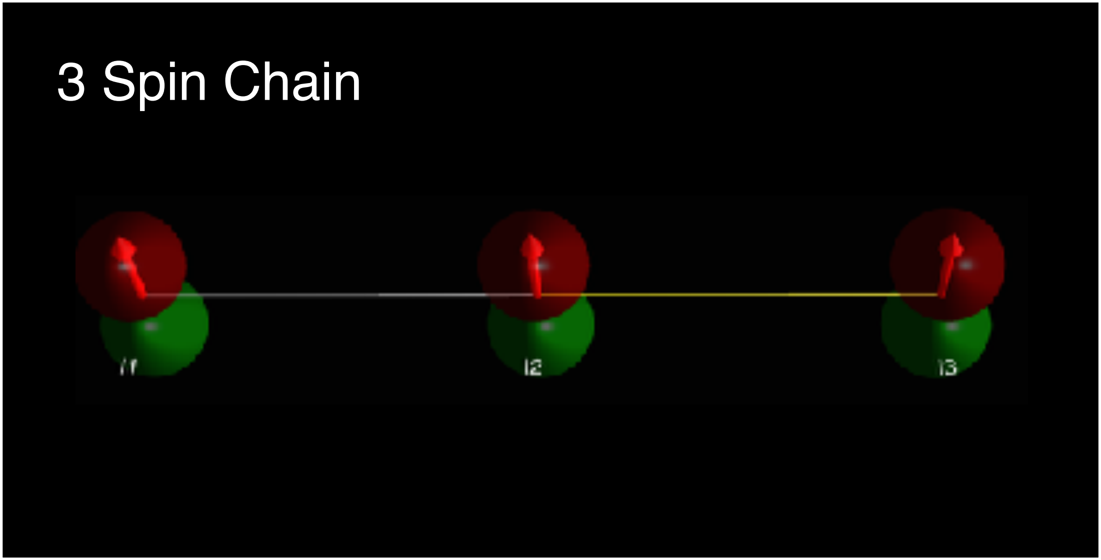
0.000 s / 1.025 s

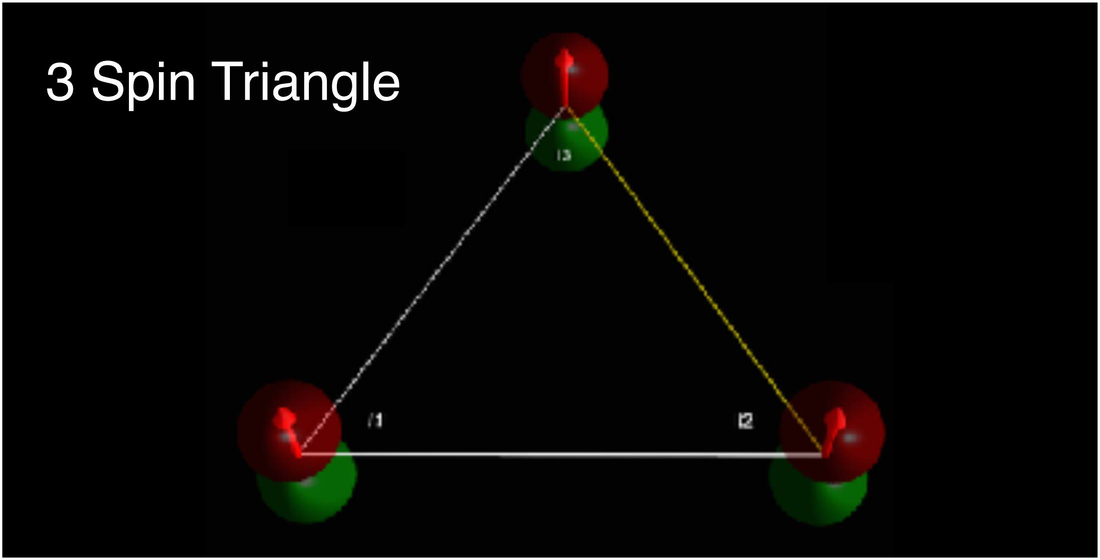
Selecting a Spin System and its Parameters (A)

By default, the option “*3 Spin Triangle*” is selected, which can always be used for systems consisting of up to three coupled spins. However, for applications involving only a single spin, two spins or a three spin chain (with no coupling between the first and the third spin), the display can be simplified using the options *1 Spin*, *2 Spins*, or *3 Spin Chain*, respectively.


1 Spin


2 Spins

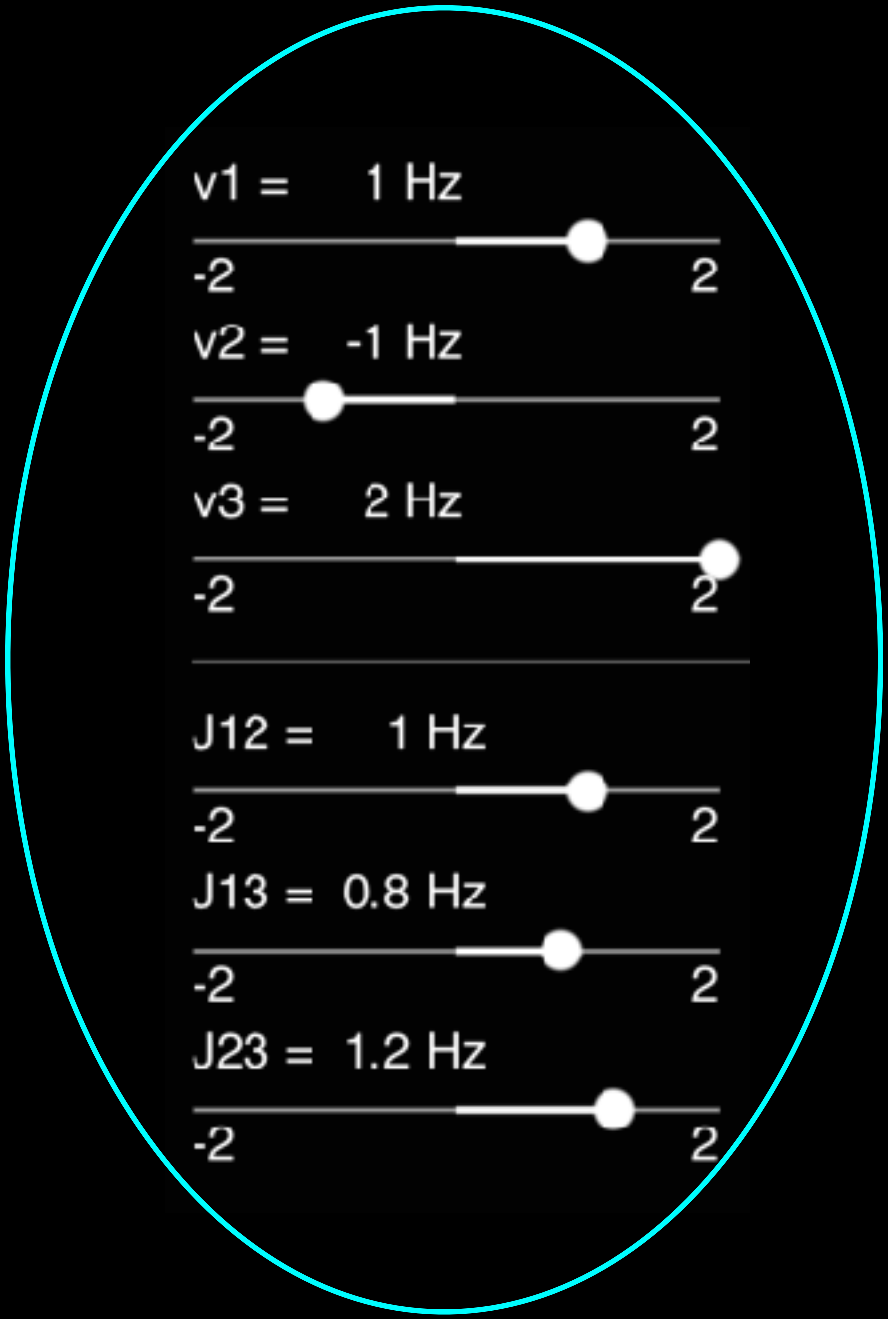

3 Spin Chain


3 Spin Triangle

Selecting a Spin System and its Parameters (B)

The spin system parameters (frequencies v and couplings J) can be inspected and modified in a control panel that can be opened in the menu *Spin System > Parameters*. (To close the panel, select *Spin System > Hide Parameters*.)

The offset frequencies v_1, v_2, v_3 and the coupling constants J_{12}, J_{13}, J_{23} can be adjusted using the sliders. In the current version of *SpinDrops*, only the range of ± 2 Hz is available for these parameters. This ensures that the spin dynamics is fluent for typical frame rates of mobile devices. In the default mode, only discrete values of the parameters can be set by the sliders in steps of 0.1 Hz. This makes it easier to set a slider e.g. to a value of exactly 0 Hz. However, it is also possible to set the parameter values continuously by selecting *Display Options > Slider Steps > Smooth*.



v1 = 1 Hz

v2 = -1 Hz

v3 = 2 Hz

J12 = 1 Hz

J13 = 0.8 Hz

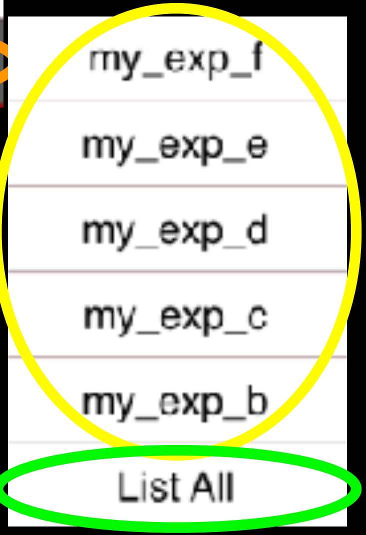
J23 = 1.2 Hz

Saving and Reading Simulation Projects

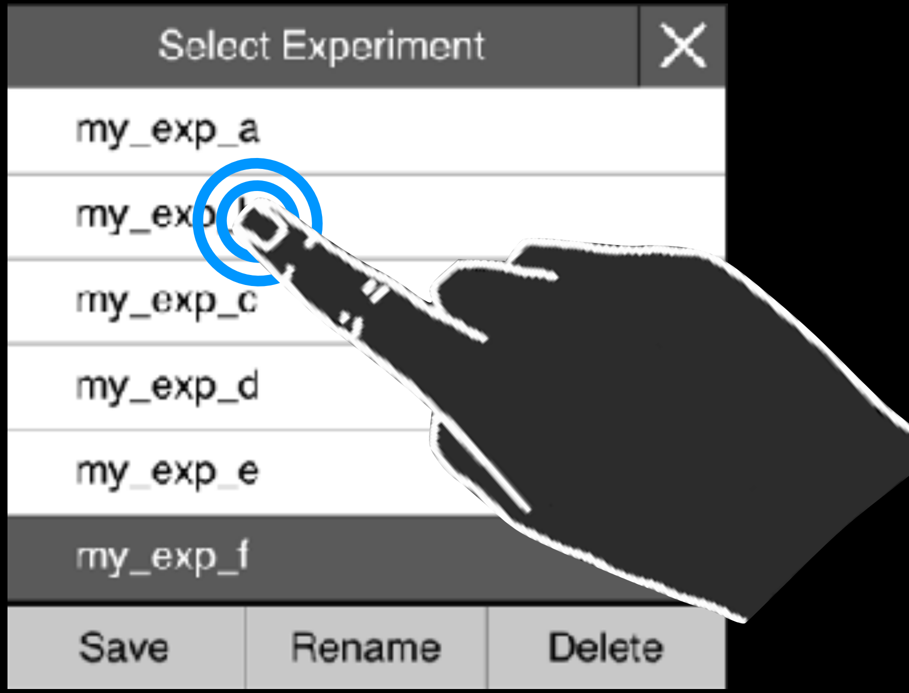
The buttons *Save Experiment* and *Read Experiment* allows you to store and retrieve all the necessary information for the simulation an experiment:

- the spin system and its parameters (frequencies ν and couplings J),
- the initial state,
- the pulse sequence.

Selecting *Read Experiment* displays the names of the five most recently used experiments of your library, which can be chosen by a *single tap*.



To see all entries of your own library of experiments, touch “List All”. If not all entries fit on one page, the list can be scrolled by a swipe. From this list, an experiment can be selected by a *double tap*. The list can be closed by touching the “X”.

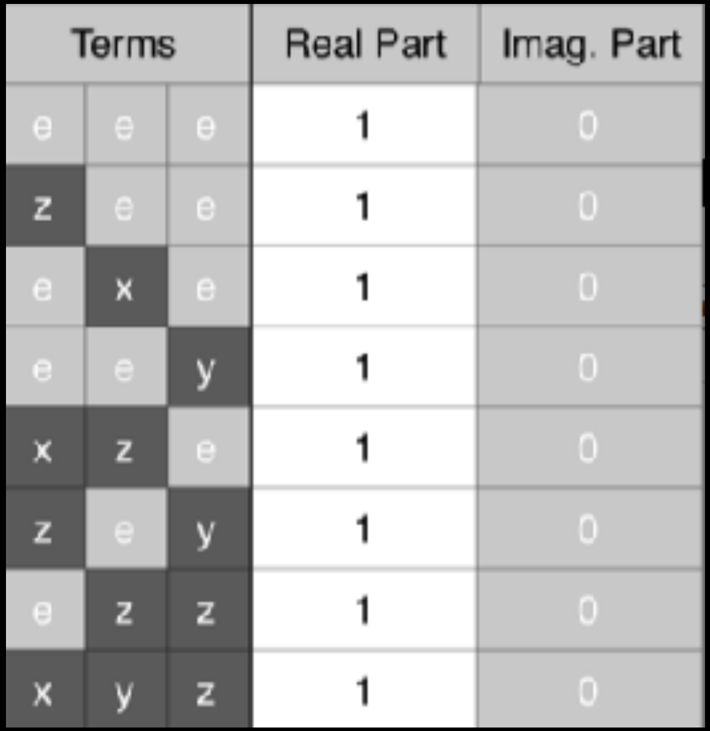


By using the buttons at the bottom of the list of experiments, it is also possible to *save* the current experiment and to *rename* or to *delete* an experiment from the list.

Shorthand Notation for Cartesian Product Operators

In the menu *Initial State > Edit Operator* and the display panel *Display Options > List Prod. Ops.*, the following shorthand notation is used for Cartesian product operators:

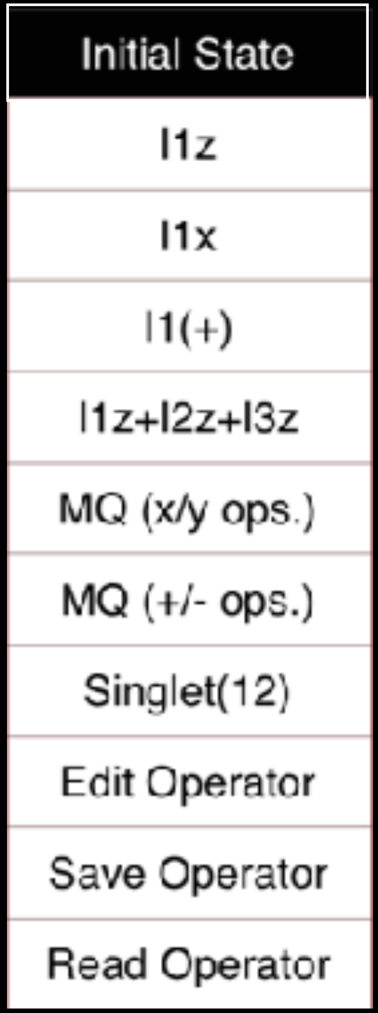
eee= 1/2 E, i.e. 1/2 times the identity operator,
zee = I_{1z},
exe = I_{2x},
eey = I_{3y},
xze = $2I_{1x}I_{2z}$,
zey = $2I_{1z}I_{3y}$,
ezz = $2I_{2z}I_{3z}$,
xyz = $4I_{1x}I_{2y}I_{3z}$



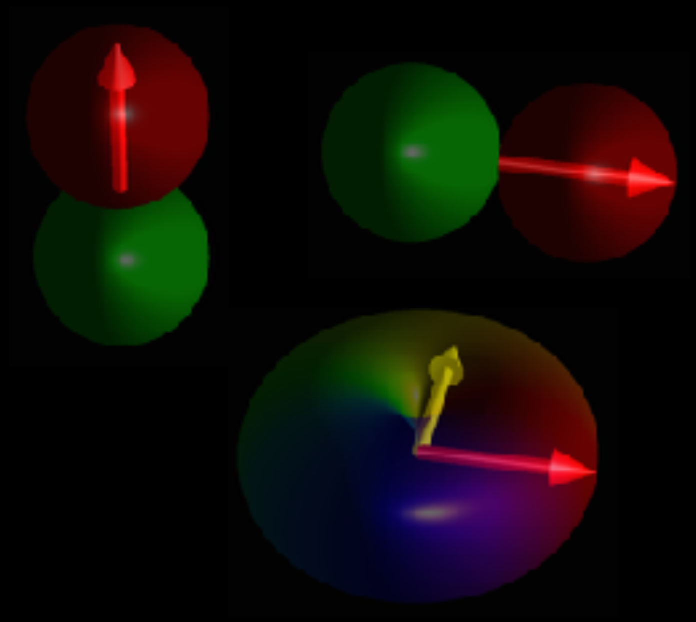
Terms			Real Part	Imag. Part
e	e	e	1	0
z	e	e	1	0
e	x	e	1	0
e	e	y	1	0
x	z	e	1	0
z	e	y	1	0
e	z	z	1	0
x	y	z	1	0

Here, the letters “x”, “y” and “z" represent the individual Cartesian spin operators I_x, I_y and I_z and the position of each letters indicates the spin it is associated with. The letter “e” represents the identity operator for a given spin. The standard prefactors (“1/2” for the identity operator E, “1” for linear operators, “2” for bilinear terms, and “4” for trilinear terms) are absorbed in the shorthand notation. In order to emphasize the spin operators I_x, I_y and I_z, the letters “x”, “y” and “z" are displayed on a dark grey background, whereas the terms “e” are displayed with a light grey background in the list displayed on the right.

Defining the Initial State (A)



The *Initial State* of the spin system is defined by choosing one of the options in the corresponding menu. The default initial state is *I1z*, corresponding to *z* magnetization of the first spin.



In addition, the following commonly used initial states can be chosen:
I1x: *x* magnetization of the first spin,
I1(+): $I_1^+ = I_{1x} + \mathrm{i}\, I_{1y}$,
and total z magnetization (*I1z+I2z+I3z* in the case of a three-spin system).

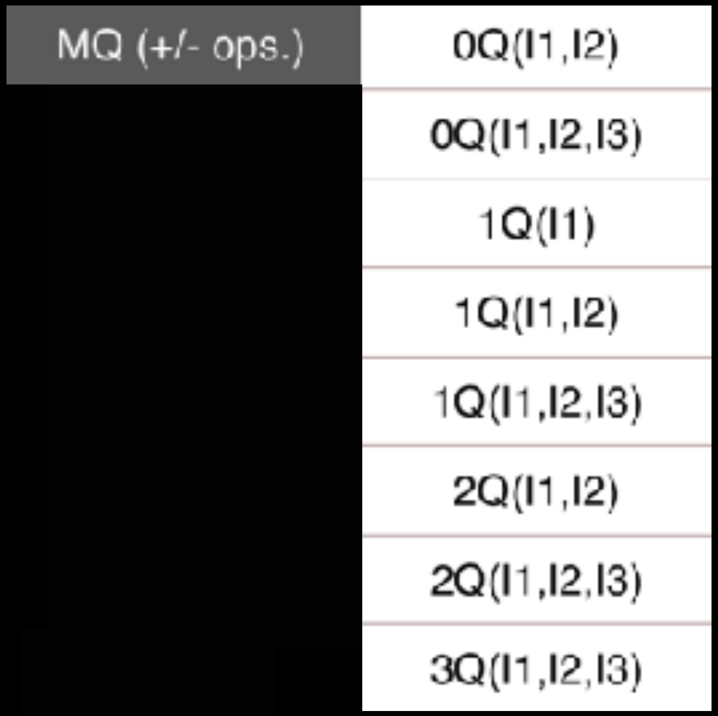
The option *MQ (x/y ops.)* provides a selection of multiple-quantum operators with quantum order ±p based on *real* combinations of Cartesian product operators.

The option *MQ (+/– ops.)* provides a selection of multiple-quantum operators with a unique quantum order p based on raising and lowering operators.

The option *Singlet(12)* provides the traceless part ($I_{1x}I_{2x}+I_{1y}I_{2y}+I_{1z}I_{2z}$) of the singlet state involving the first and second spin.

The option *Edit Operator* opens a new menu that allows you to change the initial density operator and to define any desired operator (see the following pages). An edited operator can also be stored and retrieved by using the options *Save Operator* and *Read Operator*, respectively.

Defining the Initial State (B): Multiple-Quantum Operators Based on Cartesian Product Operators



0Q(I1,I2): Zero-quantum operators involving the first and second spin.
0Qx(I1,I2), x component of the zero-quantum operator involving spins I_1 and I_2: $I_{1x}I_{2x}+I_{1y}I_{2y}$
0Qy(I1,I2), y-component of the zero-quantum operator involving spins I_1 and I_2: $I_{1y}I_{2x}-I_{1x}I_{2y}$

0Q(I1,I2,I3): Zero-quantum operators involving three spins.

1Q(I1): ± 1-quantum coherence of the first spin (I_{1x}, I_{1y})

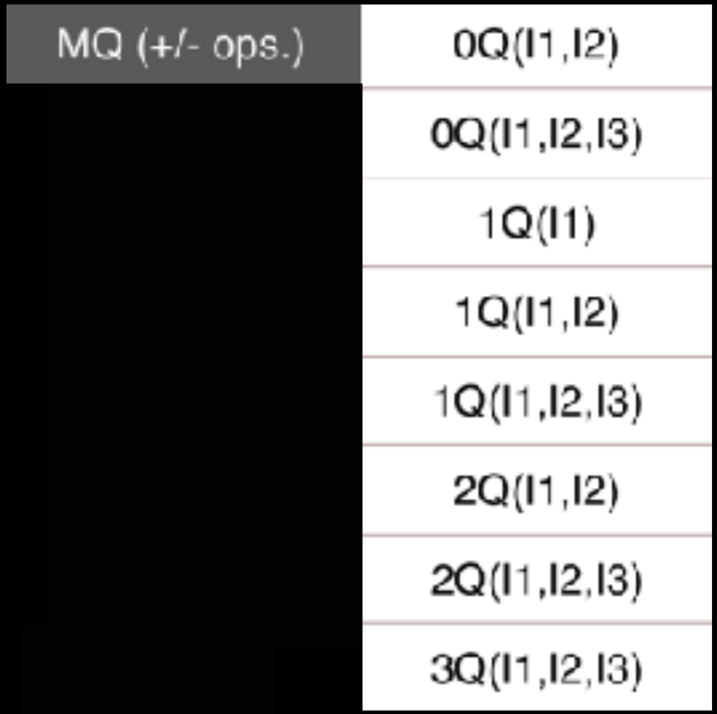
1Q(I1,I2) and *1Q(I1,I2,I3)*: ± 1-quantum operators of two and three spins, respectively.

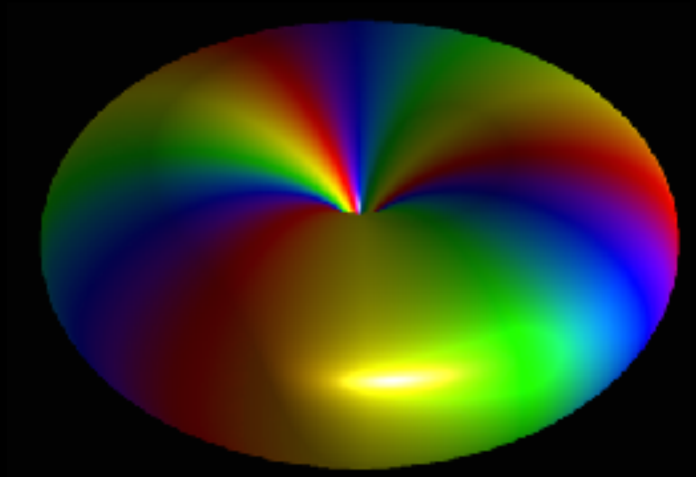
2Q(I1,I2) and 2Q(I1,I2,I3): ± 2-quantum operators.

3Q(I1,I2,I3): ± 3-quantum operators involving three spins.

Tip: In order to see how the chosen operator is defined in terms of Cartesian product operators, select *Display Options > List Prod. Ops.*

Defining the Initial State (C): Multiple-Quantum Operators with Defined Coherence Order Using I^+ and I^- Operators





0Q(I1,I2): Zero-quantum operators involving the first and second spin.

*I1(+)*I2(–)*, zero-quantum operator $I_1^+I_2^-$ involving spins I_1 and I_2.

*I1(–)*I2(+)*, zero-quantum operator $I_1^-I_2^+$ involving spins I_1 and I_2.

0Q(I1,I2,I3): Zero-quantum operators involving three spins.

1Q(I1): +1 or –1-quantum coherence of the first spin (I_1^+, I_1^-)

1Q(I1,I2) and *1Q(I1,I2,I3)*: +1 or –1-quantum operators of two and three spins, respectively.

2Q(I1,I2) and 2Q(I1,I2,I3): +2 or –2-quantum operators.

3*Q(I1,I2,I3)*: +3 or –3-quantum operators.

Tip: In order to see how the chosen operator is defined in terms of Cartesian product operators, select *Display Options > List Prod. Ops.*

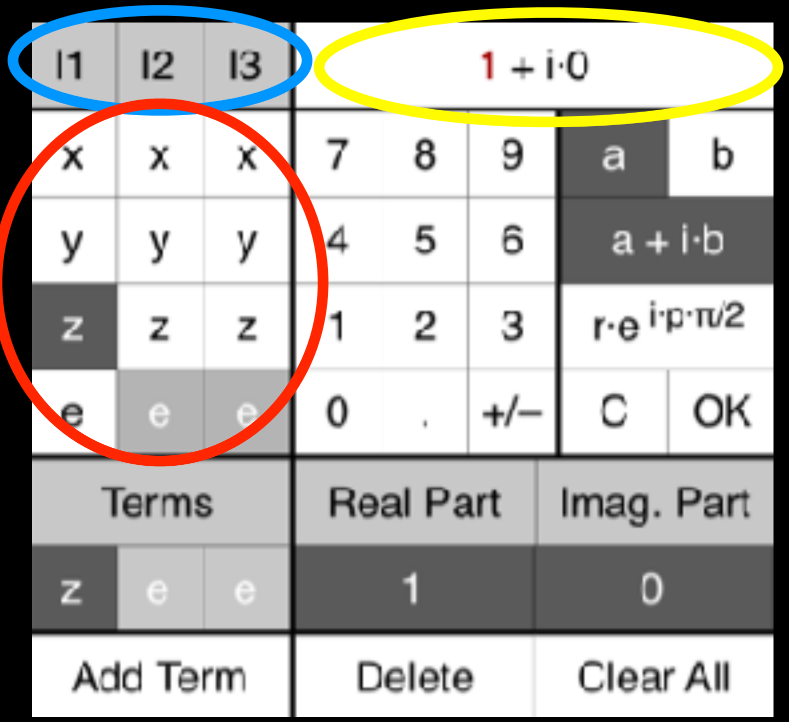
Defining the Initial State (D): Edit Operator

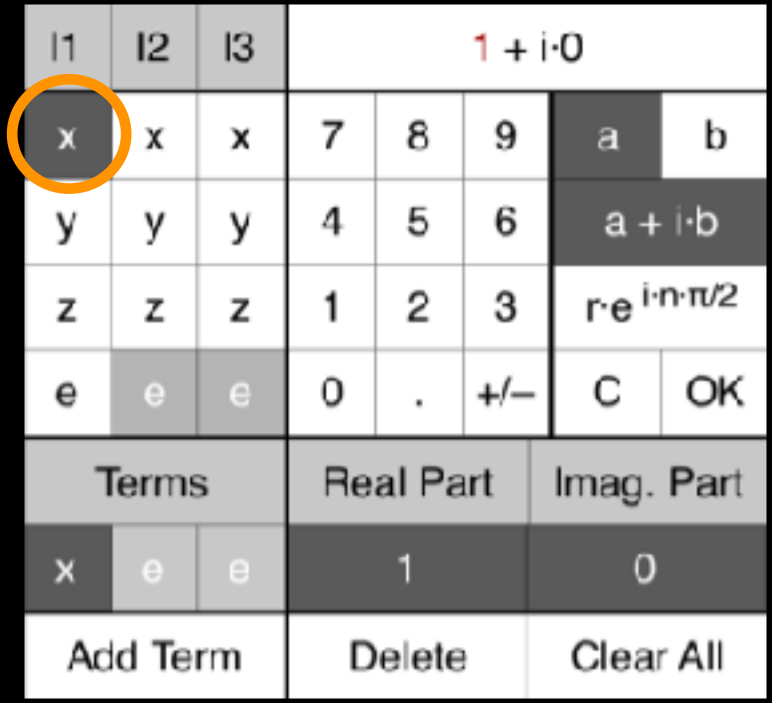
The current initial state of the spin system can be edited and hence any desired initial state can be defined in the input panel *Initial State > Edit Operator*.

The display on the right shows the input panel after opening it, when the current initial state is I_{1z} (i.e. zee in our shorthand notation).

In the upper left part of the input panel, Cartesian product operators can be defined using the button x, y, z, and e, (highlighted by a red ellipse) where the columns labeled *I1*, *I2*, and *I3* (blue ellipse) correspond to the first, second and third spin, respectively. The complex prefactor ($1 + i\cdot 0$) of the currently edited product operator term is shown in the display window at the top (yellow ellipse). By default, the prefactors are displayed in the form $a + i\cdot b$, where a and b are the real and imaginary parts, respectively. (Alternatively, the complex prefactors can be defined in terms of the radial part r and the phase $\phi=n\cdot\pi/2$ by activating the button $r\cdot e^{i\cdot n\cdot\pi/2}$.)

For example, I_{1z} can be changed to I_{1x} by touching x in the first column. Note that also the corresponding droplet in the DROPS display will change instantly.





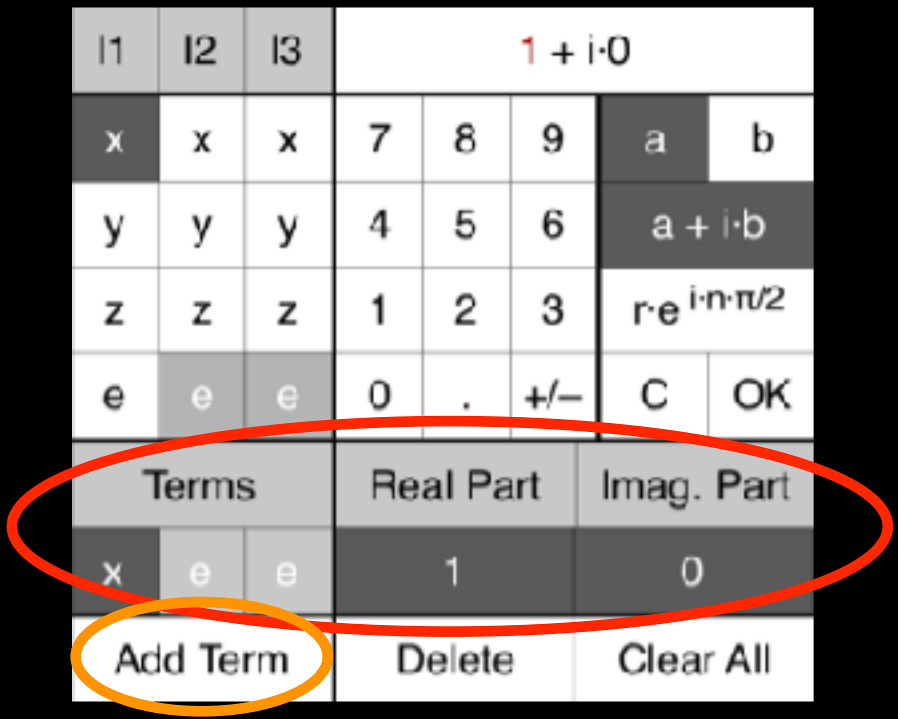
Defining the Initial State (E): Edit Operator

The currently defined product operator terms of the initial density operator are listed at the bottom of the panel (red ellipse). In the example shown at the right, the initial state consists only of the term xee. The real and imaginary parts of the corresponding prefactor are 1 an 0, respectively, i.e. the first term is simply I_{1x}.

Additional terms can be added by touching the button *Add Term* (orange ellipse). By default, this creates the new term (1 + i·0)·eee (short-hand notation for the identity operator). For example, in order to define the initial operator $I_1^+ = I_{1x} + \mathrm{i}\ I_{1y}$, change the second term from eee to yee and its prefactor from (1 + i·0) to (0 + i·1).

In order to change the prefactor (1 + i·0) to (0 + i·1) in the "*a + i·b*" mode (yellow ellipse), cancel the real part "*a*" using the *C* button, activate the imaginary part by touching the *b* button and touch 1. (Alternatively, you could activate the "$r{\cdot}e^{i \cdot n \cdot \pi/2}$" mode and set *n* to 1).

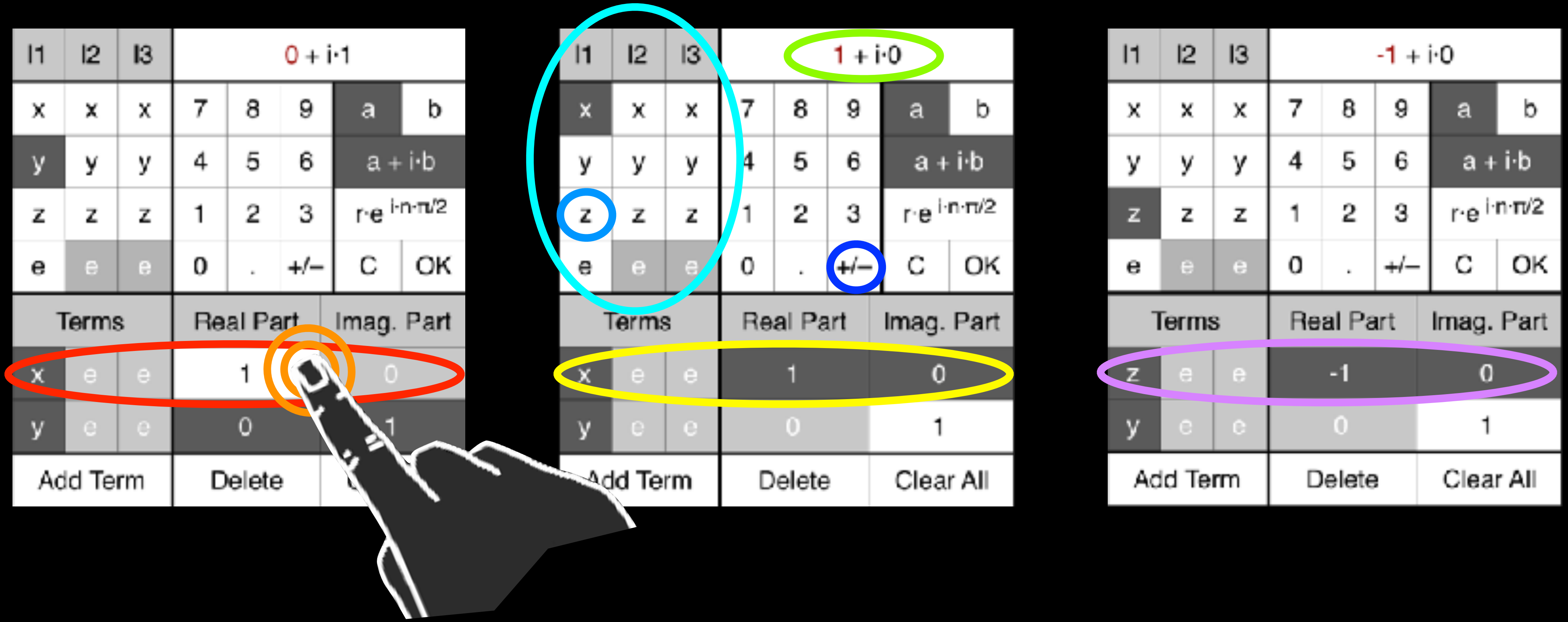
Now the initial density operator is set to $I_{1x} + \mathrm{i}\ I_{1y}$, with the first product operator term (1 + i·0)·xee and the second term (0 + i·1)·yee (green ellipse).



Terms	Real Part	Imag. Part
x e e	1	0

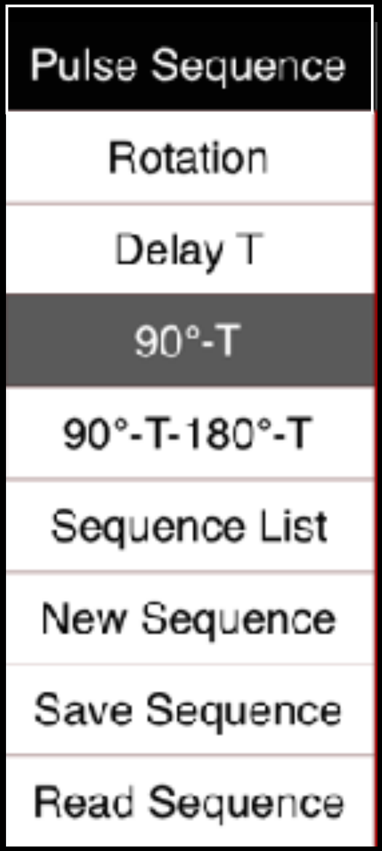
Terms	Real Part	Imag. Part
x e e	1	0
y e e	0	1

Defining the Initial State (F): Edit Operator



In the list of operator terms displayed at the bottom of the panel, you can activate and modify any desired term by a *double tap*. In the list, the real and imaginary parts of the prefactor of the activated term are highlighted by a white font on a dark grey background. The Cartesian product operator components and the prefactor of the activated term can be edited using the input panel. To cancel an activated term, touch the *Delete* button.

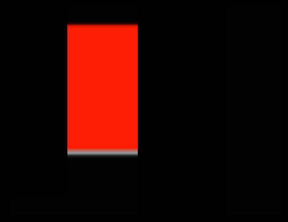
For example, to change the operator I_{1x} + i I_{1y} defined on the previous page to $-I_{1z}$ + i I_{1y}, double tap the first term (red ellipse). This activates the first term (yellow ellipse) and displays its current prefactor and product operator components in the input panel. Touching the *z(I1)* and the +/– buttons changes the first term from I_{1x} to $-I_{1z}$.



Selecting the Pulse Sequence (A)

The initial state of the spin system is manipulated by a *Pulse Sequence*, which can be selected or created in the corresponding menu. The chosen pulse sequence is displayed graphically at the bottom of the screen. In addition, you can display a listing of the pulse sequence elements (pulses, delays, isotropic mixing) by selecting *Display Options > List/Edit Seq*.

The default pulse sequence (*90°-T*) consists of a 90°_y pulse followed by a free evolution period T with a duration of 1 second.



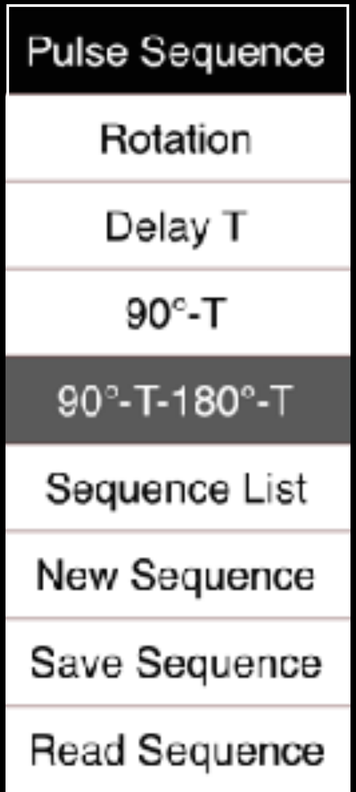
Rotation: The following options can be chosen.

  90° Pulse: A 90° pulse with a desired phase (x, y, –x, or –y) can be chosen.
  180° Pulse: A 90° pulse with a desired phase (x, y, –x, or –y) can be chosen.
  z Rotation: Here, *z* rotations of various angles can be chosen.

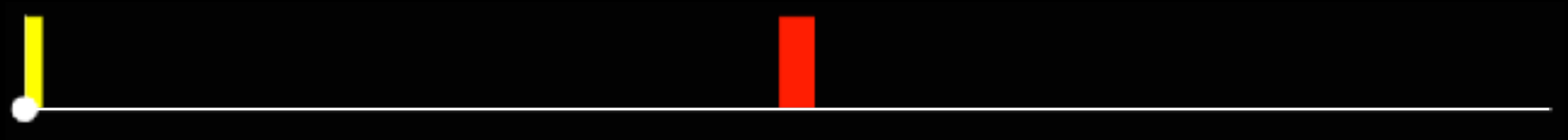
Delay T: A free-evolution delay can be chosen. The basic options are *T=1 s* (corresponding to a fixed delay of 1 second) and *T=1/(2·J12)* which defines the duration of the delay in terms of the coupling constant J_{12} between the first and the second spin.

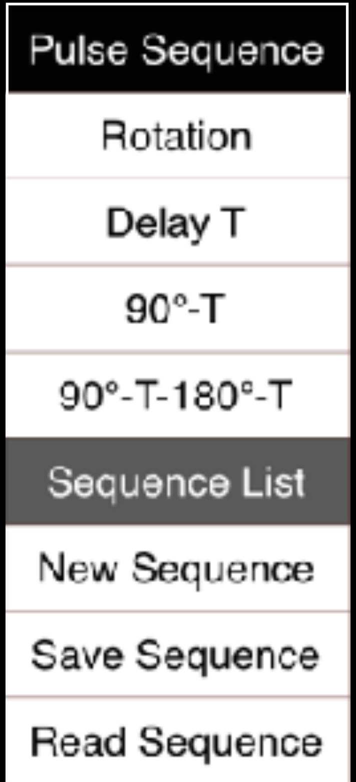
Tip 1: A new pulse sequence is only activated at the lowest menu level, i.e. when all required parameters are defined. This is confirmed by a beep.
Tip 2: As will be explained in more detail below, the pulses and delays can be easily modified by double tapping the corresponding displayed pulse sequence element.

Selecting the Pulse Sequence (B)

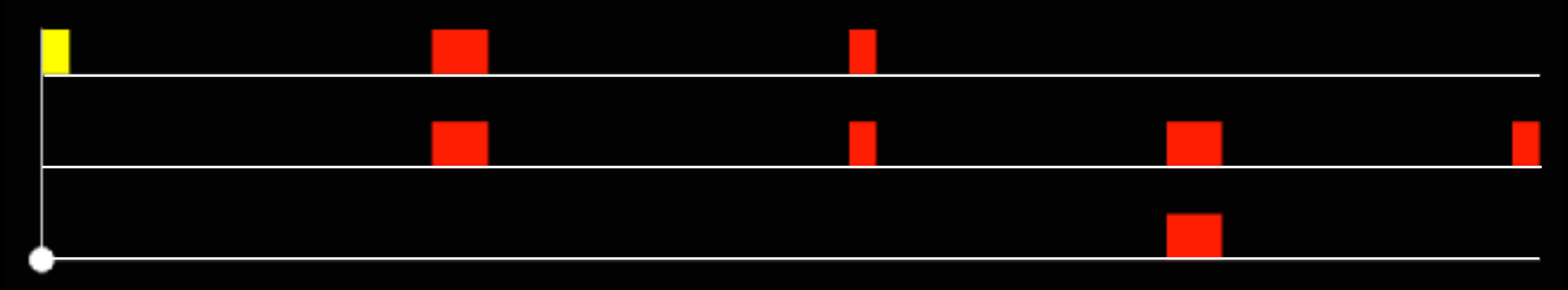


90°-T-180°-T: An echo sequence consisting of a 90°_y pulse (yellow) followed by a free evolution period *T*, a 180°_x pulse (red), and a second period *T*.





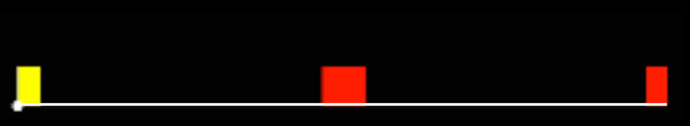
Sequence List: In this menu, entries of a list of *homonuclear* and *heteronuclear* pulse sequences can be selected.



Tip: See *Help > Color Code* for the color code used in *SpinDrops* to represent pulse phases.

Selecting the Pulse Sequence (C): Homonuclear List

Nonsel. INEPT12:



For $J_{12} \neq 0$ and $J_{13}=J_{23}=0$, this sequence of duration $1/(2J_{12})$ transfers I_{1z} (i.e. *z* magnetization of the first spin) completely to antiphase coherence $-2I_{1z}I_{2y}$.

0Q and 2Q Exc.:

For $J_{12} \neq 0$ and $J_{13}=J_{23}=0$, this sequence of duration $1/(2J_{12})$ transfers I_{1z} (i.e. *z* magnetization of the first spin) completely to $2I_{1y}I_{2x}$ (which is a mixture of 0- and ±2-quantum coherence).

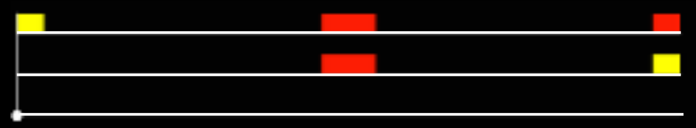
Isotropic Mix. 12:

This sequence consists of a period of selective isotropic mixing (of the first and the second spin) with a duration $1/(2J_{12})$, which transfers polarization I_{1z} via the zero-quantum term $(2I_{1x}I_{2y} - 2I_{1y}I_{2x})$ to polarization I_{2z}.

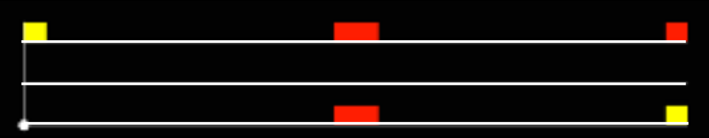
Iso-12-23-31: This sequence demonstrates a “round trip” polarization transfer of I_{1z} to I_{2z}, to I_{3z}, and back to I_{1z} using an I_1-I_2-selective isotropic mixing period of duration $1/(2 J_{12})$, followed by an I_2-I_3-selective isotropic mixing period of duration $1/(2 J_{23})$ and a final I_1-I_3-selective isotropic mixing period of duration $1/(2 J_{13})$.

Selecting the Pulse Sequence (D): Heteronuclear List

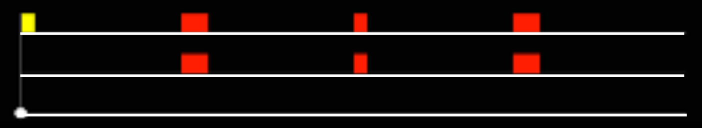
INEPT12:
If $J_{12}\neq0$, this sequence transfers I_{1z} *completely* to antiphase coherence $2I_{1z}I_{2x}$, even if $J_{13}\neq0$ and $J_{23}\neq0$.



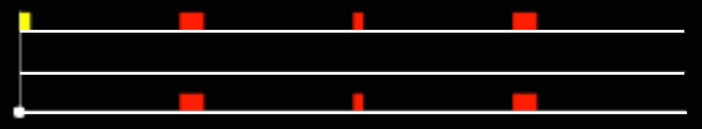
INEPT13:
If $J_{13}\neq0$, this sequence transfers I_{1z} *completely* to antiphase coherence $2I_{1z}I_{3x}$, even if $J_{12}\neq0$ and $J_{23}\neq0$.



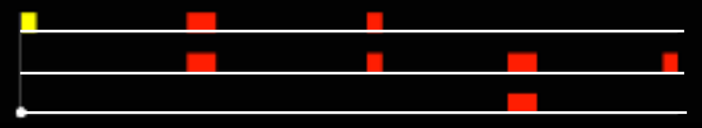
Ref. *INEPT12*:
If $J_{12}\neq0$, this refocused INEPT sequence transfers I_{1z} *completely* to I_{2x}, even if $J_{13}\neq0$ and $J_{23}\neq0$.



Ref. *INEPT13*:
If $J_{13}\neq0$, this refocused INEPT sequence transfers I_{1z} *completely* to I_{3x}, even if $J_{12}\neq0$ and $J_{23}\neq0$.

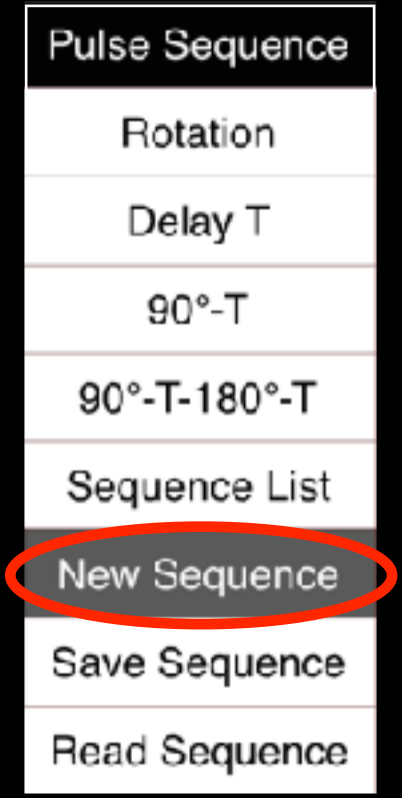


z1 -> zzz:
If $J_{12}\neq0$ and $J_{23}\neq0$, this sequence transfers I_{1z} *completely* to $4I_{1z}I_{2z}I_{3z}$.



DEPT-45, DEPT-90, DEPT-270:
See *Help > Examples > Example 5: Spectral Editing* for a more detailed discussion of the DEPT sequence.

Selecting the Pulse Sequence (E): New Sequence



Additional homonuclear or heteronuclear pulse sequences not contained in the list of predefined sequences can be created using the sequence editing tools, which are described in more detail in

Help > Sequence Editor.

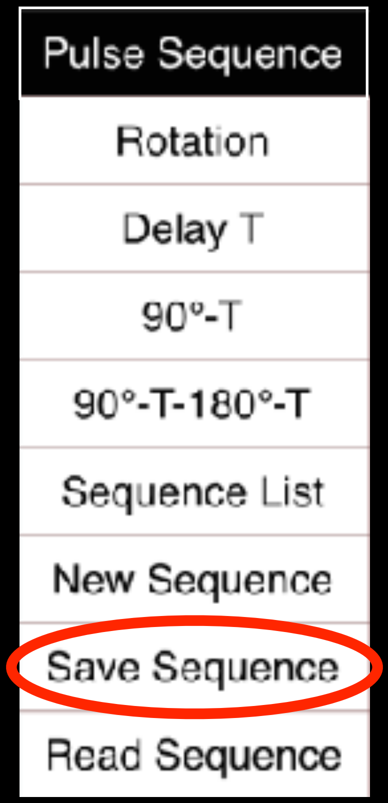
A new pulse sequence can be efficiently built from scratch by touching the *New Sequence* button (red ellipse).

Pulse Sequence > New Sequence > Homonuclear creates a new sequence list for experiments with non-selective pulses.

Pulse Sequence > New Sequence > Heteronuclear creates a new sequence list for experiments with spin-selective pulses.

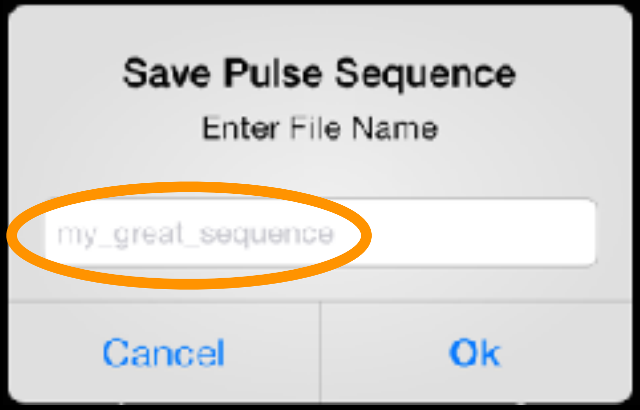
With the sequence editing tools described in *Help > Sequence Editor*, it is possible to modify existing pulse sequences. One option to edit a given pulse sequence is simply to activate one of its pulse sequence elements in the graphical pulse sequence display using a *double tap*. Alternatively, *Display Options > List/Edit Seq.* displays the list of sequence elements, which can be activated and edited by a *double tap*. Pulse sequence elements can be modified, copied, pasted, dragged, deleted and created.

Selecting the Pulse Sequence (F): Save Sequence


Pulse Sequence
Rotation
Delay T
90°-T
90°-T-180°-T
Sequence List
New Sequence
Save Sequence
Read Sequence

You can build your own sequence library.

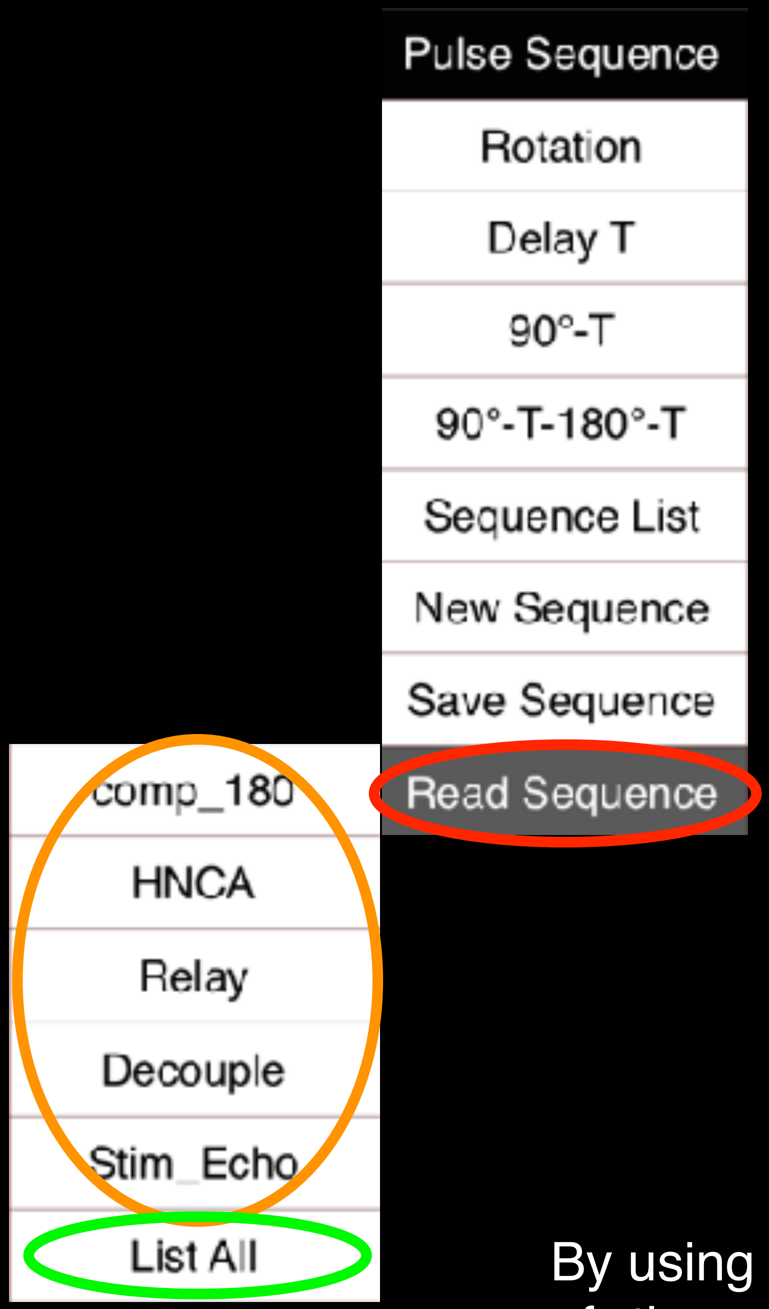
Select *Save Sequence* to store the current pulse sequence and enter a file name in the corresponding input field.

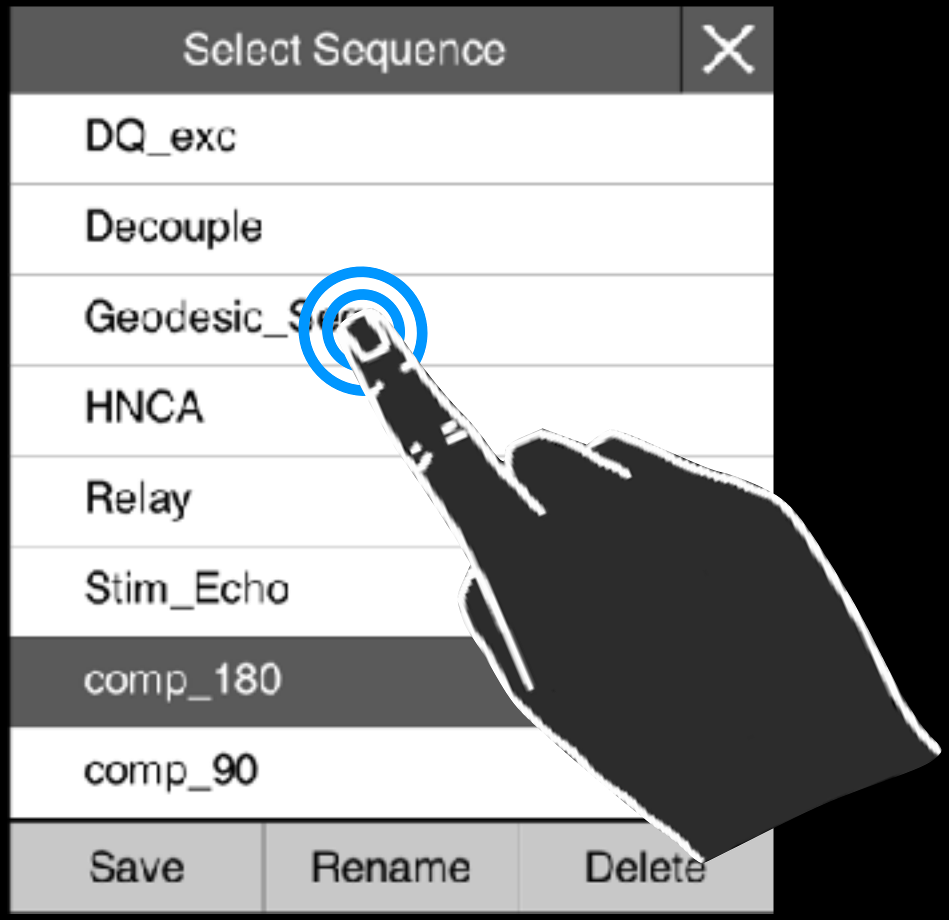

Save Pulse Sequence
Enter File Name
my_great_sequence
Cancel
Ok

Selecting the Pulse Sequence (G): Read Sequence

Selecting *Read Sequence* displays the names of the five most recently used pulse sequences of your library, which can be chosen by a single tap.

To see a list of all entries of your own pulse sequence library, touch “List All”. If not all entries fit on one page, the list can be scrolled by a swipe. From this list, a sequence can be selected by a double tap. The list can be closed by touching the “X”.



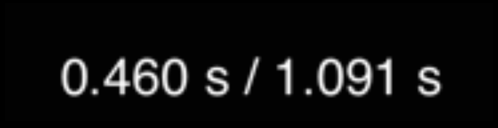


By using the buttons at the bottom of the sequence list, it is also possible to save the current sequence and to rename or to delete a sequence from the list.

Controlling the Simulations (A)

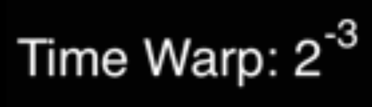
The buttons below the pulse sequence interactively control the simulation of the spin dynamics:

■	Stop and return to the beginning of the pulse sequence
▶ / ⏸	Play/Pause
⏵ / ⏩	Slower/Faster
⏭ / ⏮	Skip to the end/beginning of the current pulse or delay
🔁̸ / 🔁	Repeat mode off/Repeat mode on



0.460 s / 1.091 s

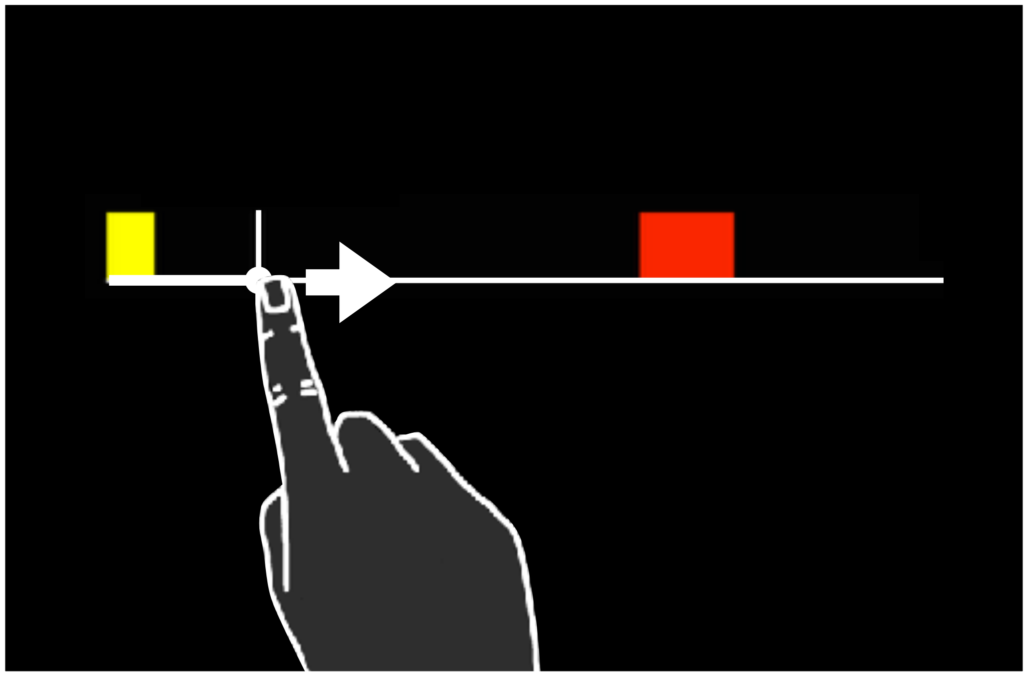
At the right of the control buttons, the current time (here 0.460 s) and the total duration of the pulse sequence (here 1.091 s) is displayed (iPad only).

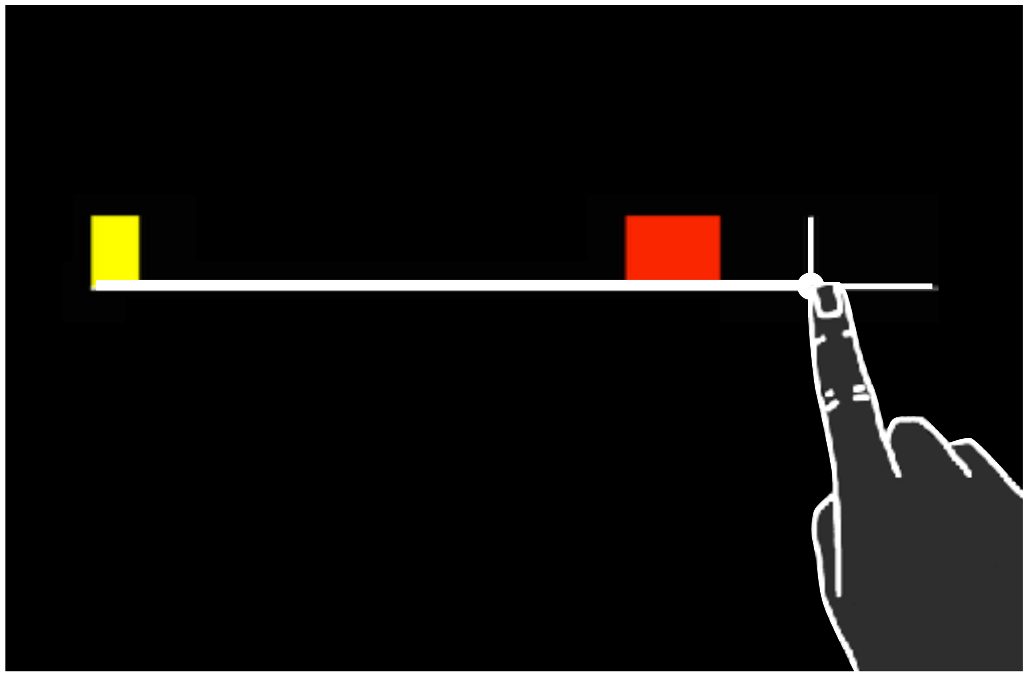


Time Warp: 2^{-3}

When a simulation is running, the acceleration factor (“*Time Warp*”) is displayed at the left of the control buttons (iPad only). For example, an acceleration factor of 2^{-3} indicates that the simulation is slowed down by a factor of $2^{-3} = 1/2^3 = 1/8$. Touching the *Slower* or *Faster* button decreases or increases the acceleration by a factor of 1/2 or 2, respectively.

Controlling the Simulations (B)





The white dot and the attached vertical line indicate the current time point of the simulation. As explained on the previous page, the current time point can be controlled using the control buttons at the bottom of the sequence plot.

It is also possible to control the time evolution directly by touching and dragging the white dot to the desired position.

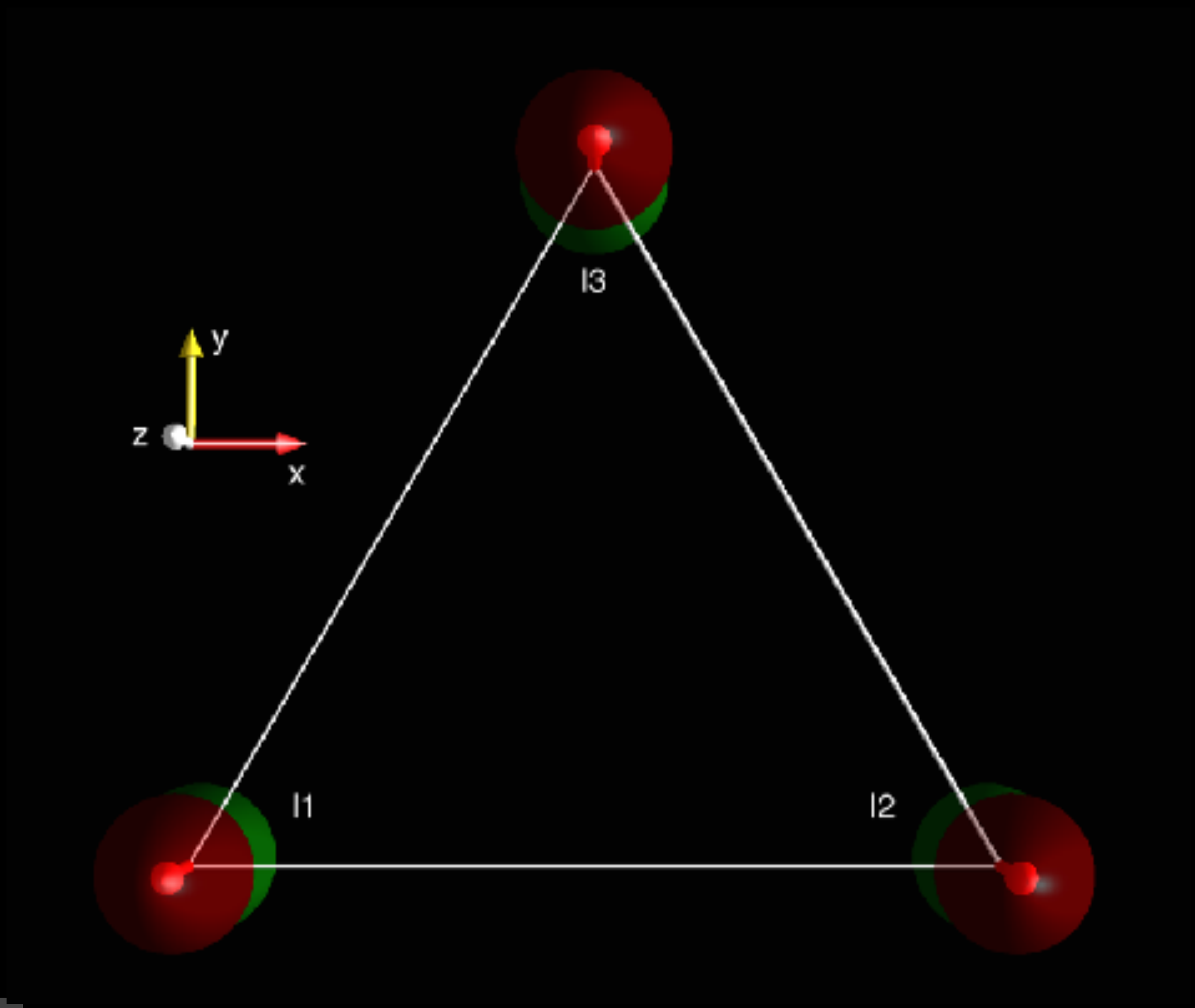
This allows you to precisely control the speed with which the DROPS display is changed during the pulse sequence.

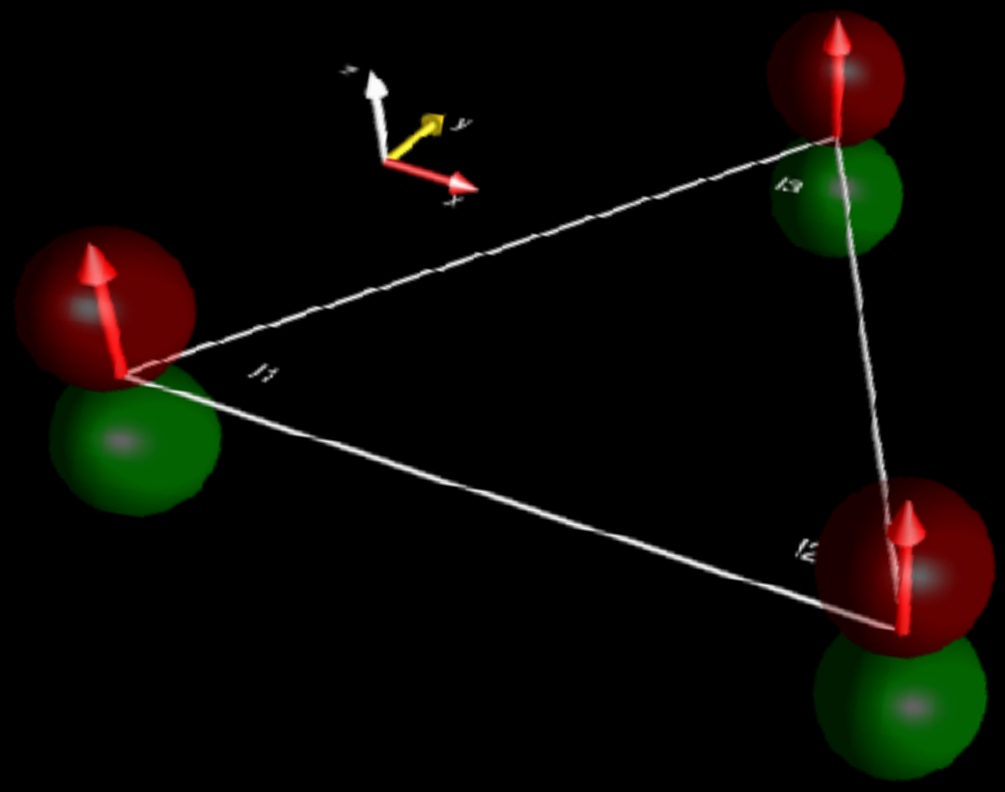
For an even finer control, the pulse sequence display can be zoomed by pinching with two fingers.

Tip: The simulation should be stopped or paused when the current time point is moved manually.

Manipulating the DROPS Display (A)

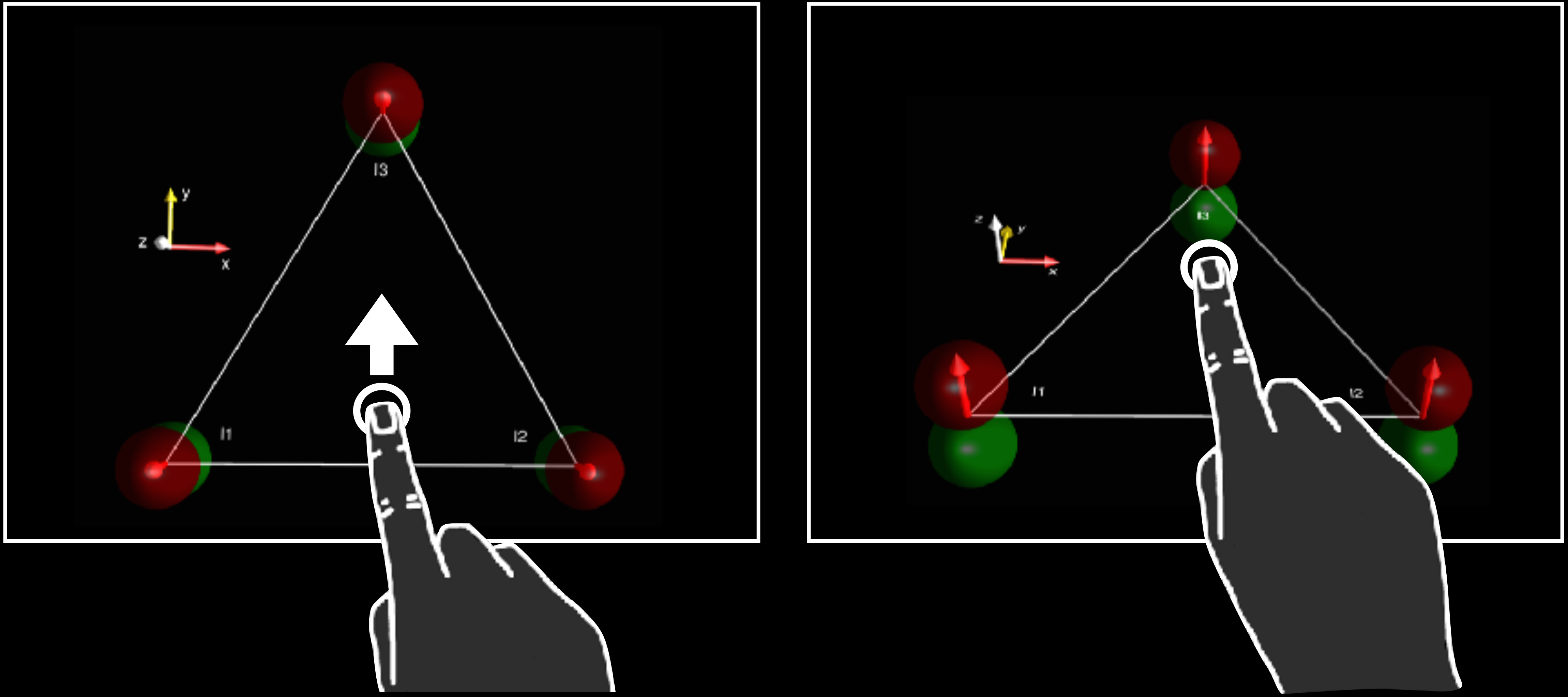
To view the three-dimensional shapes of the droplets from different perspectives, you can *rotate*, *shift* and *zoom* the DROPS display with one- or two-finger gestures (as illustrated on the following pages). It is also possible to change the view angle by tilting the device (*Display Options > Enable Parallax*).





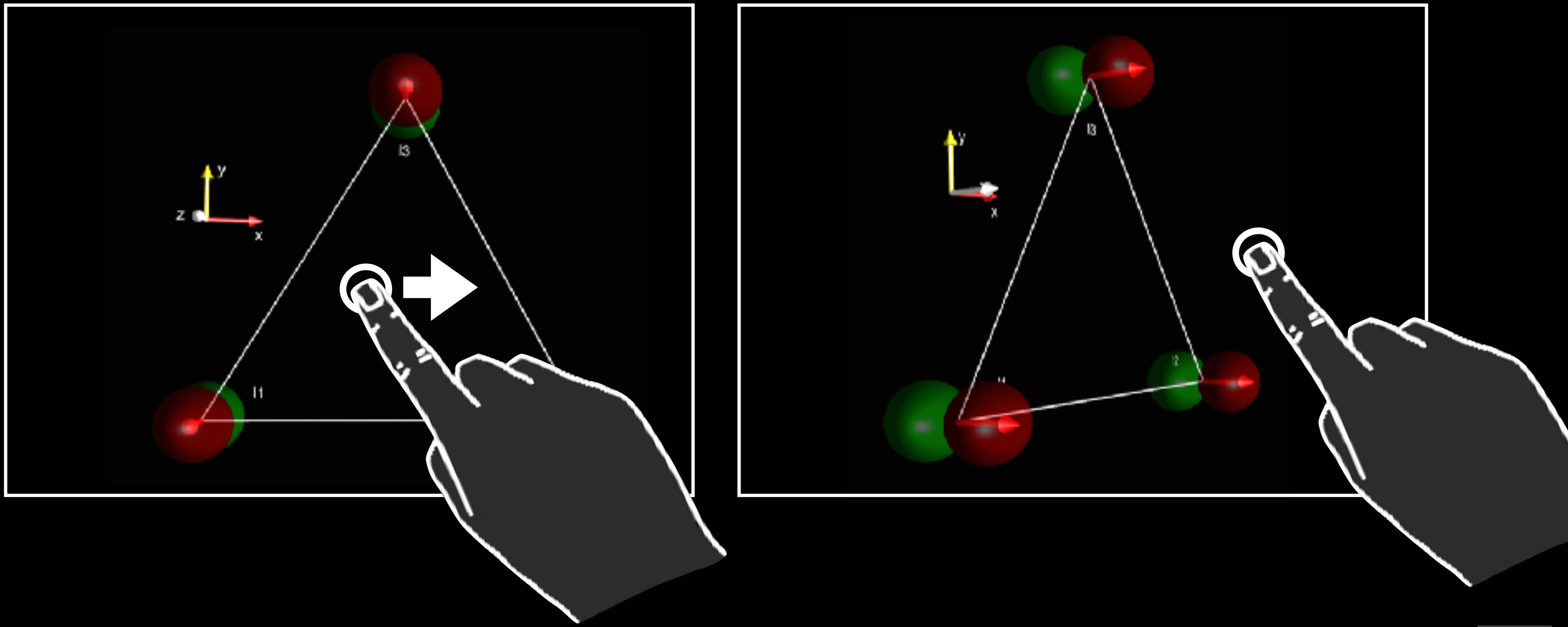
Manipulating the DROPS Display (B)

The DROPS display can be rotated like a trackball by dragging one finger. In the example shown below, the DROPS display is rotated around the horizontal axis of the screen by dragging the finger upwards.



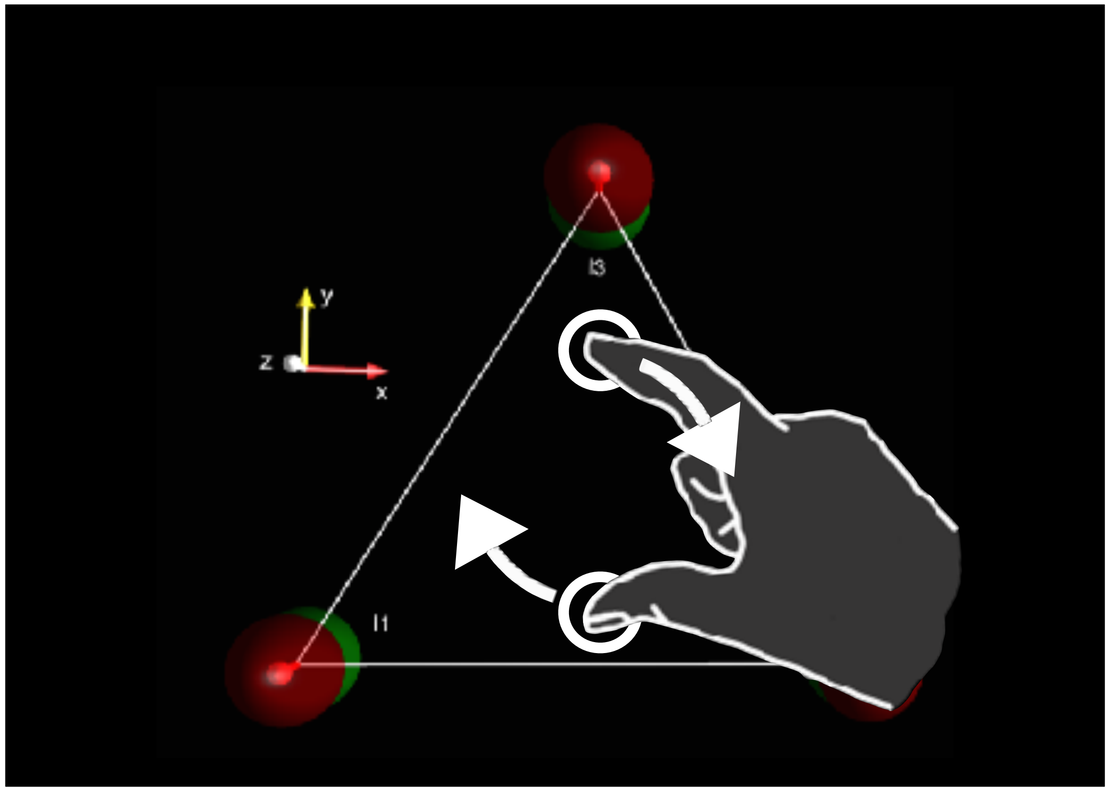
Manipulating the DROPS Display (C)

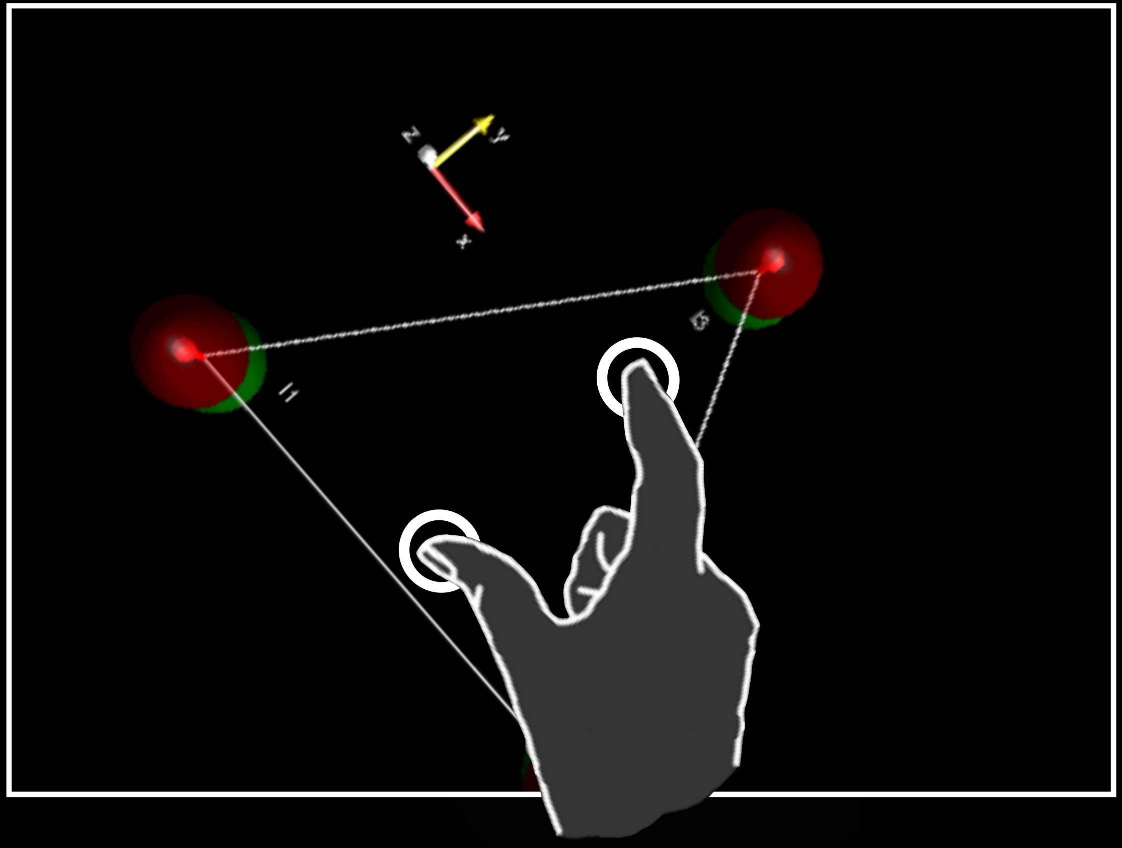
The DROPS display is rotated like a trackball around the vertical axis of the screen by dragging the finger from left to right.



Manipulating the DROPS Display (D)

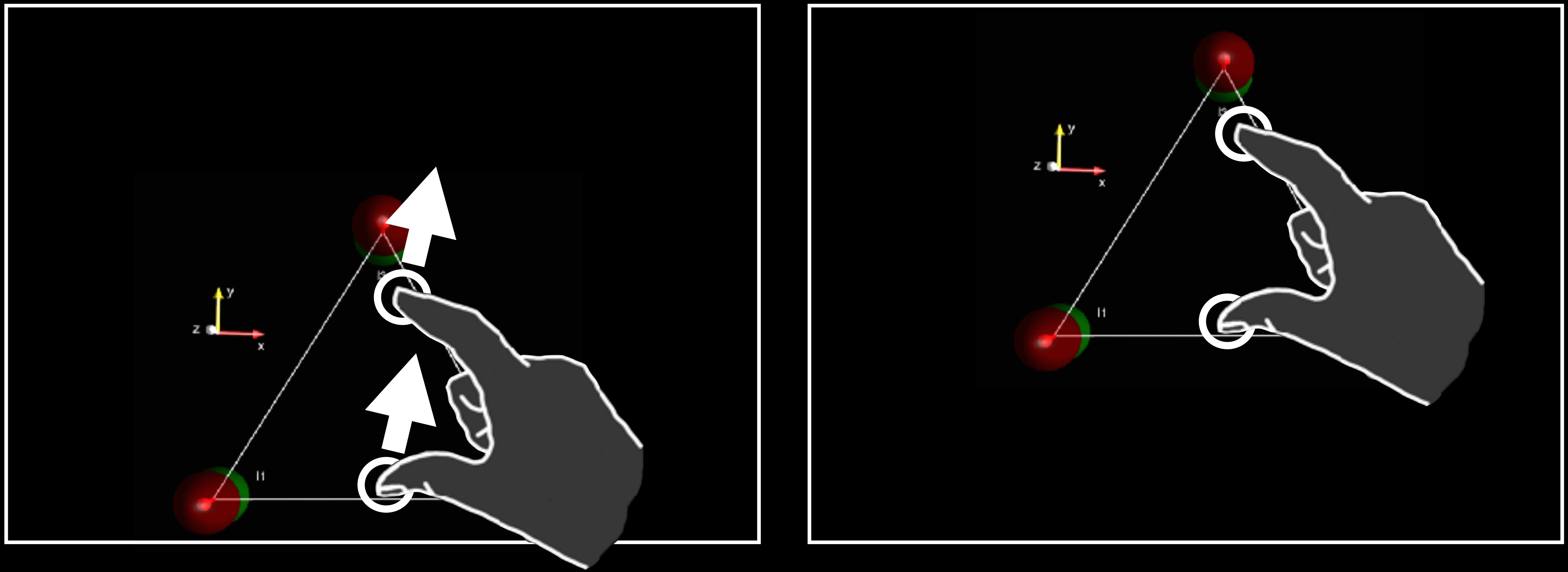
Rotate like a steering wheel in the plane of the screen by twisting two fingers in a circular motion.





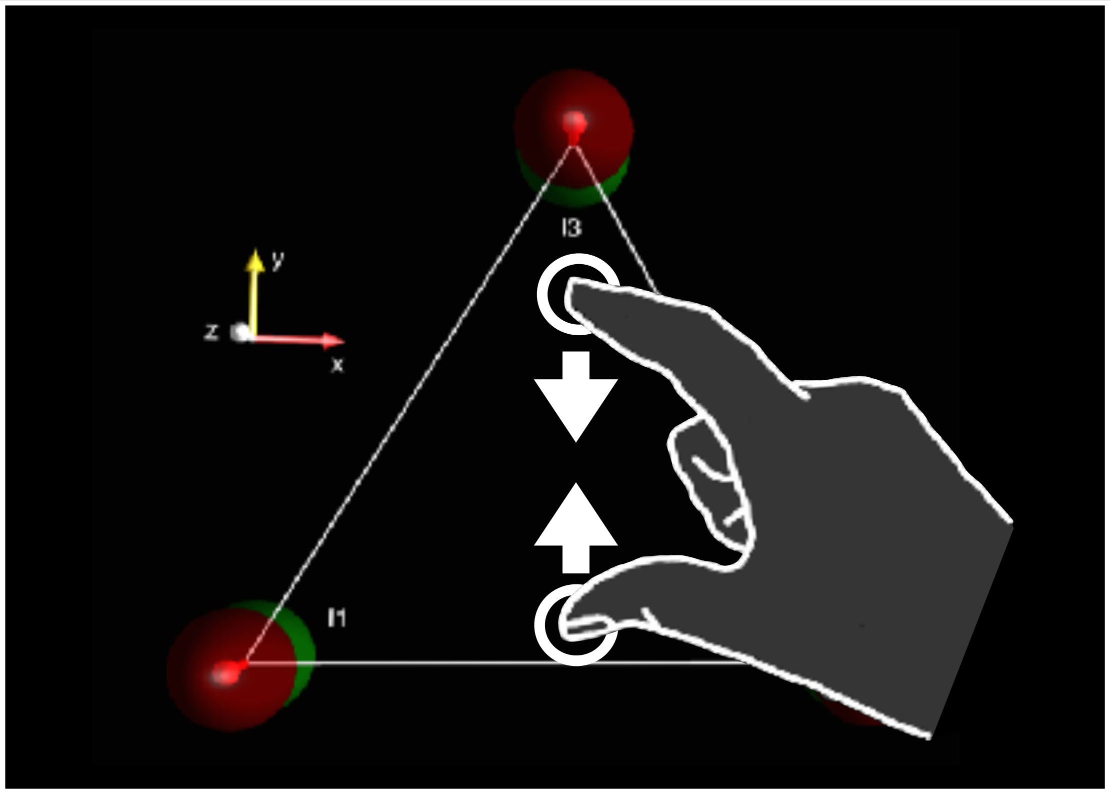
Manipulating the DROPS Display (E)

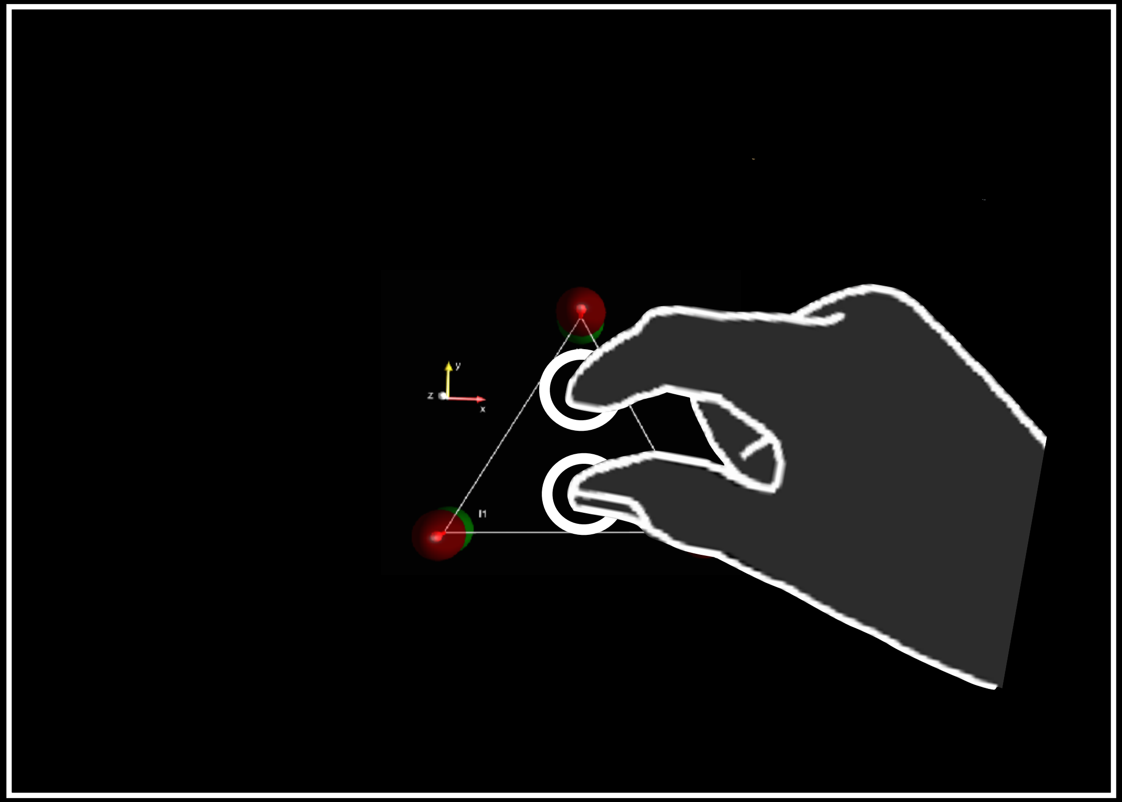
Shift in the plane of the screen by dragging with two fingers.



Manipulating the DROPS Display (F)

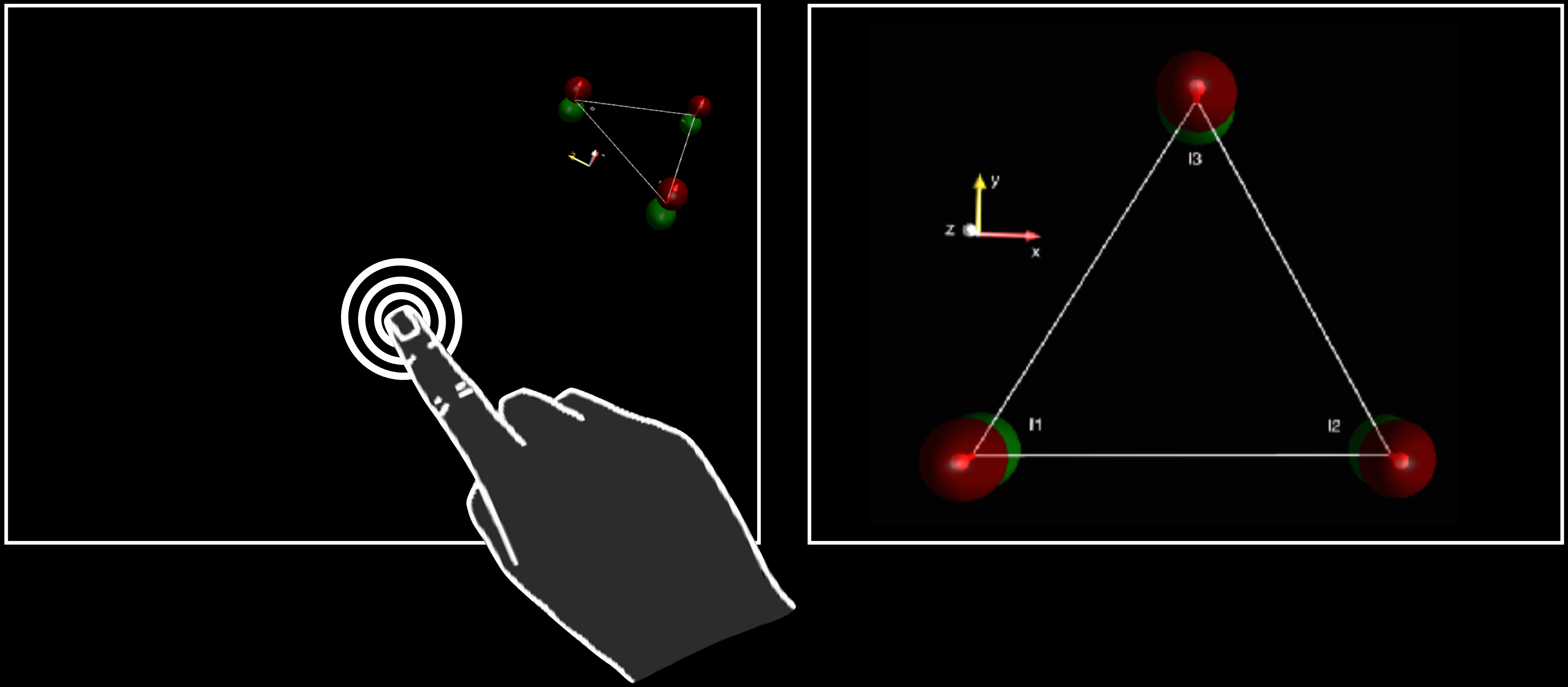
Zoom in and out with two fingers. Pinching your fingers together makes the image smaller and spreading the fingers apart enlarges the image.





Manipulating the DROPS Display (G)

Restore the default view of the DROPS representation by performing a triple tap with one finger.

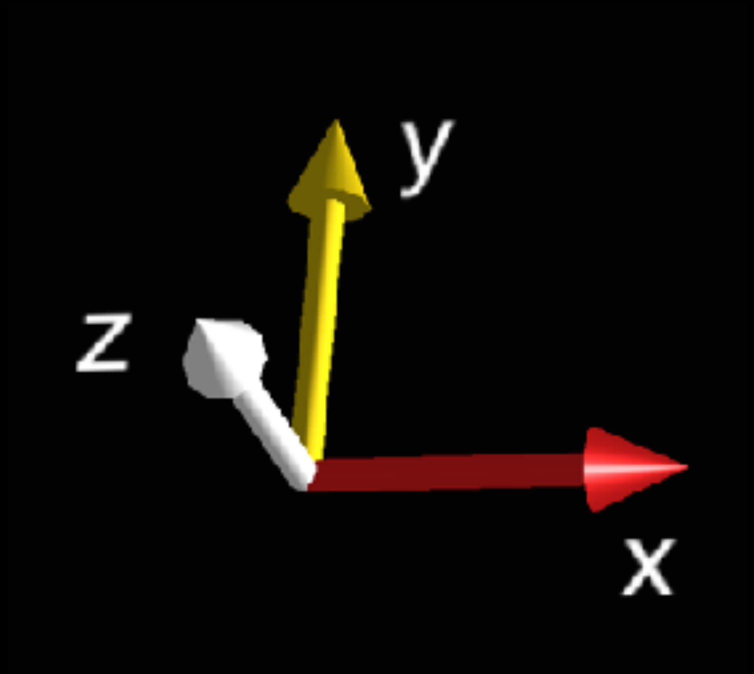


Coordinate System

In the DROPS display, a coordinate system is usually shown for reference. The axes of the coordinate system are labelled x, y, and z and in addition, the following colors are used to easily distinguish the axes:

Yellow: y axis

White: z axis



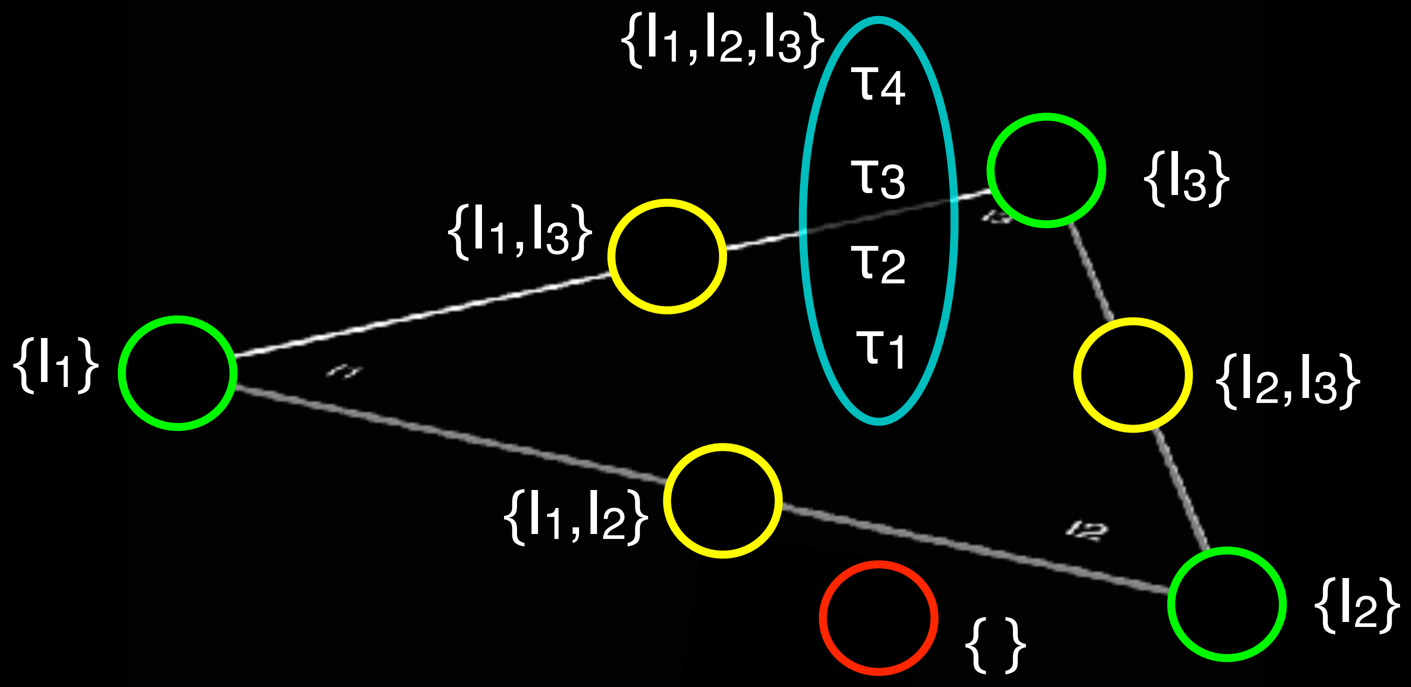
Red: x axis

DROPS Display for a *Three-Spin Triangle* (A)

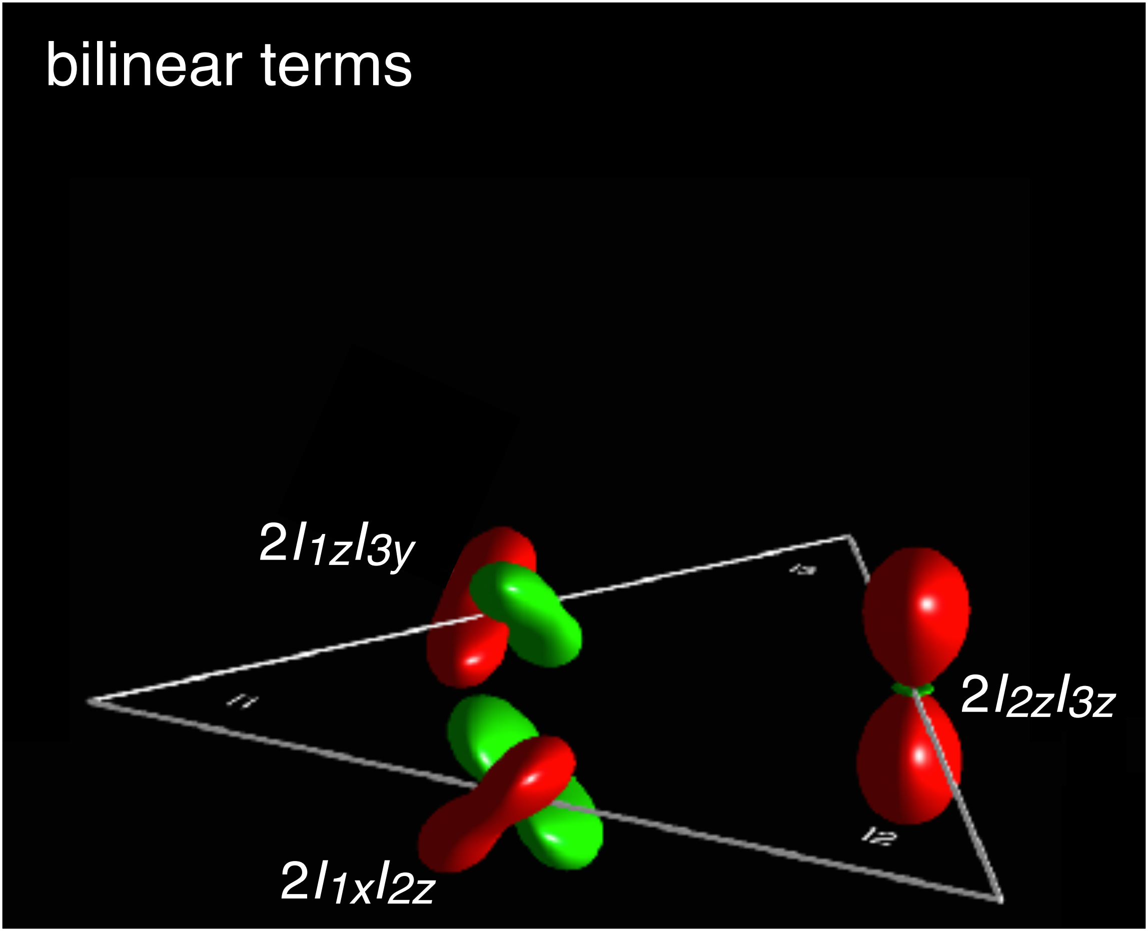
In the standard DROPS display based on the LISA basis, the location of a *droplet* indicates the set of involved spins. The following locations are used in the default setting:

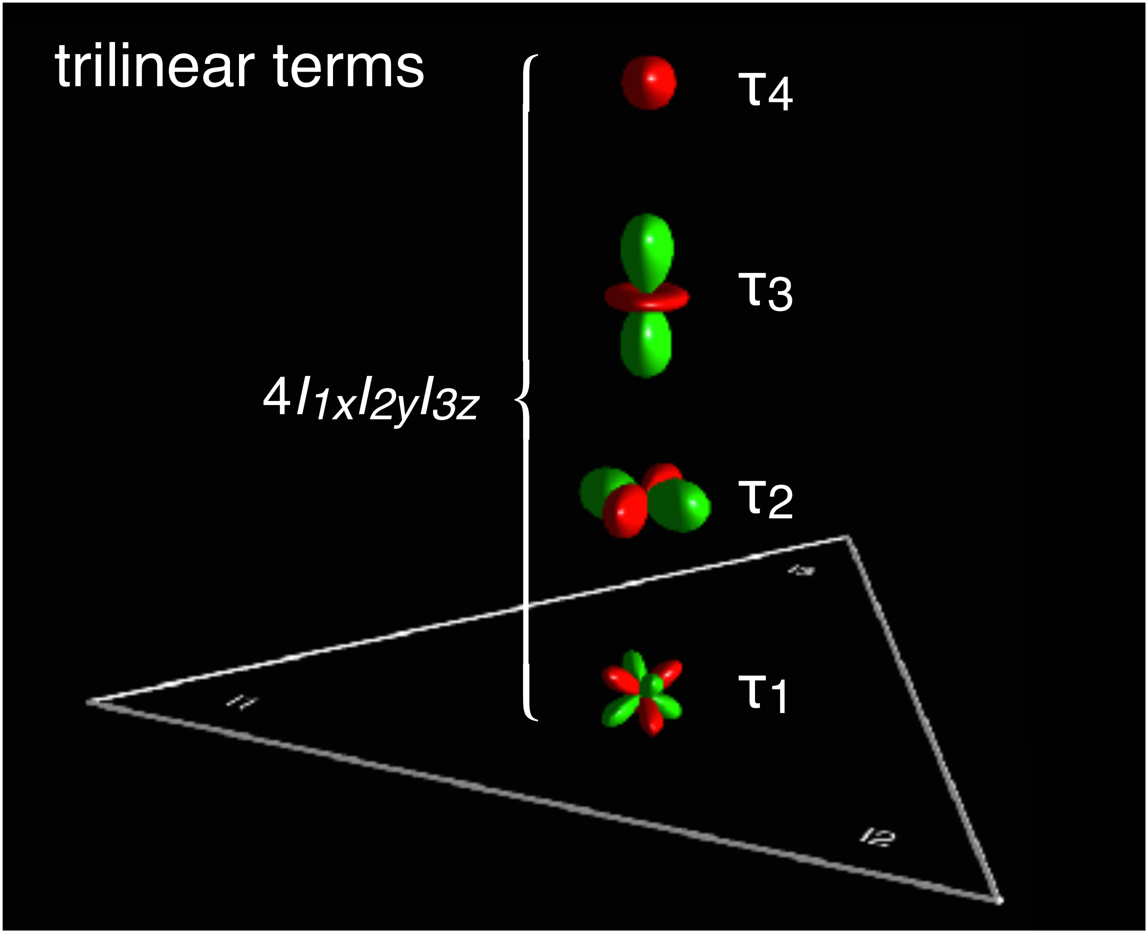
- Droplets corresponding to product operator terms involving only a single spin operator (*linear terms)* are located at the *corners* of a triangle. Each corner is labeled to indicate with which spin (I_1, I_2, or I_3) it is associated.
- Droplets corresponding to *bilinear terms* are located on the corresponding *edges* of the triangle.
- Droplets corresponding to *trilinear terms* are located in the *center* and *above* the triangle.
- The droplet representing a term which involves *no spin operator* (i.e. which is proportional to the *identity operator*) is located *below* the triangle.

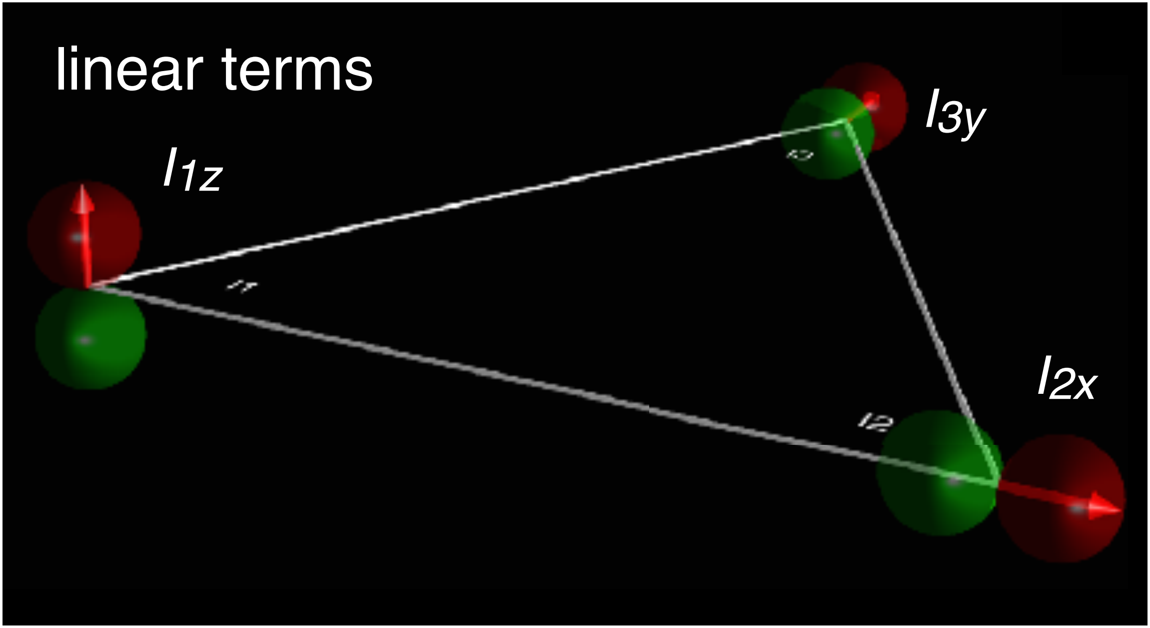
Examples of the DROPS display for linear, bilinear and trilinear terms and the identity operator are shown on the next page.

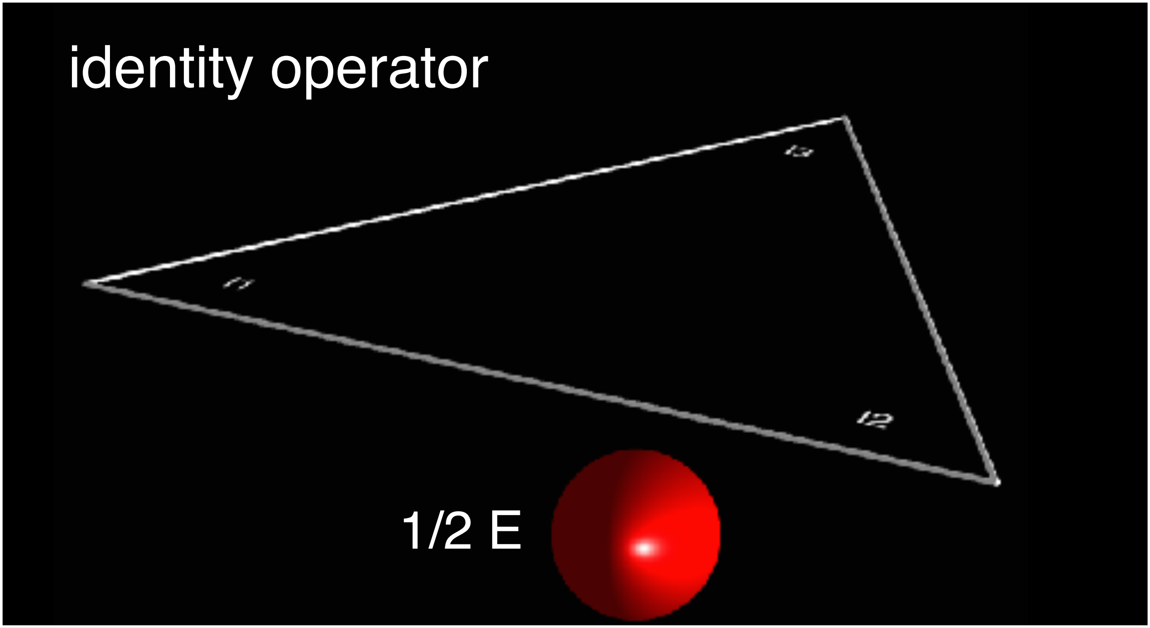


DROPS Display for a *Three-Spin Triangle* (B)


bilinear terms

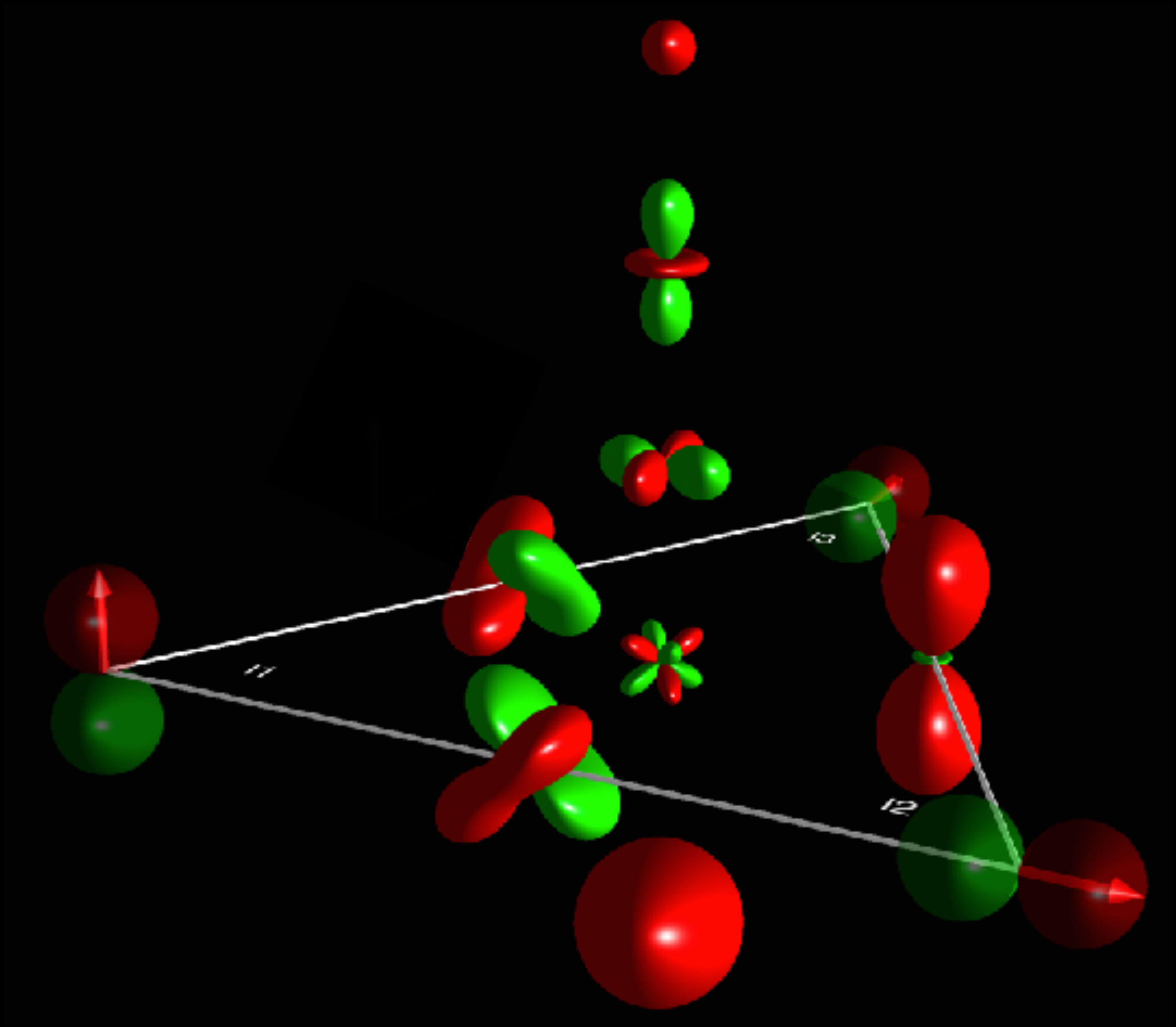

trilinear terms


linear terms


identity operator

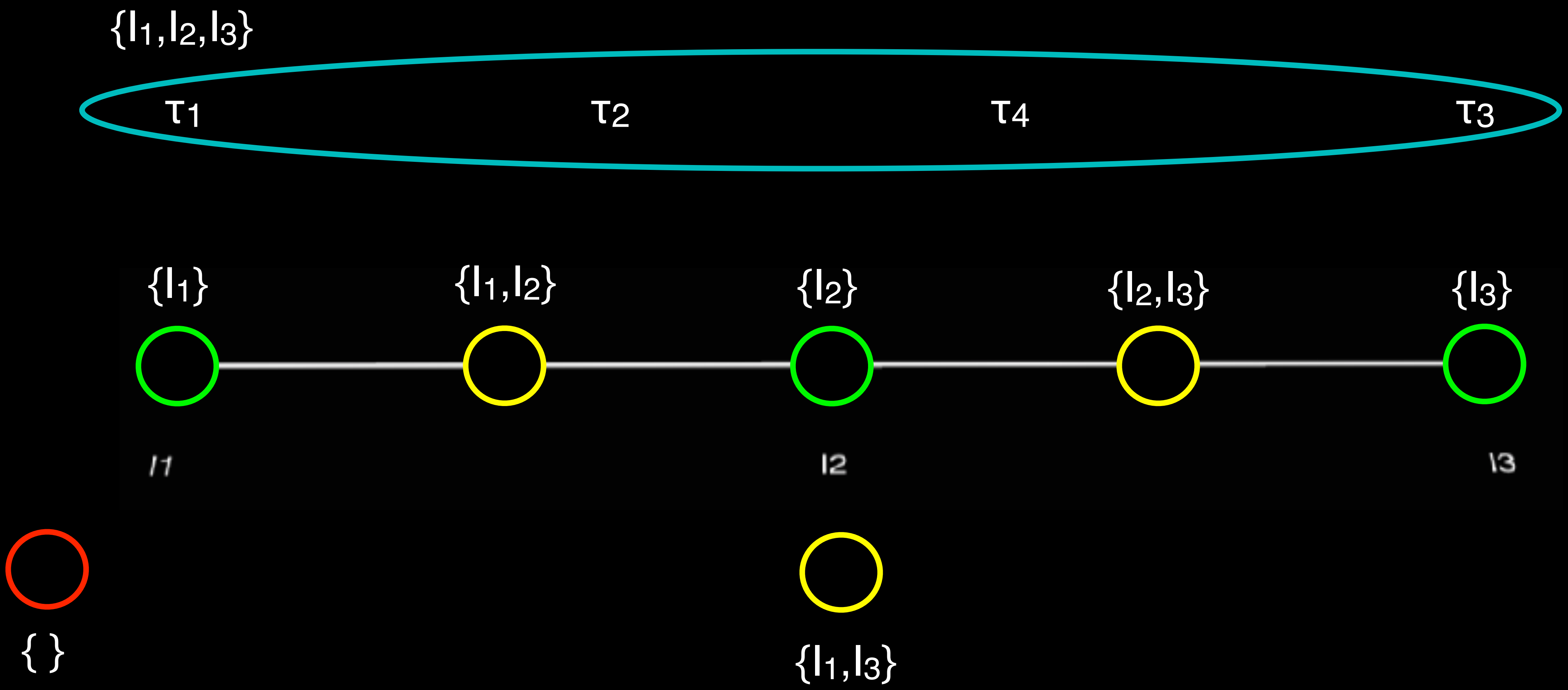
DROPS Display for a *Three-Spin Triangle* (C)

On the previous page, the linear, bilinear and trilinear terms as well as the term proportional to the identity operator term were shown separately. In the standard DROPS display, these terms are shown simultaneously in one figure.



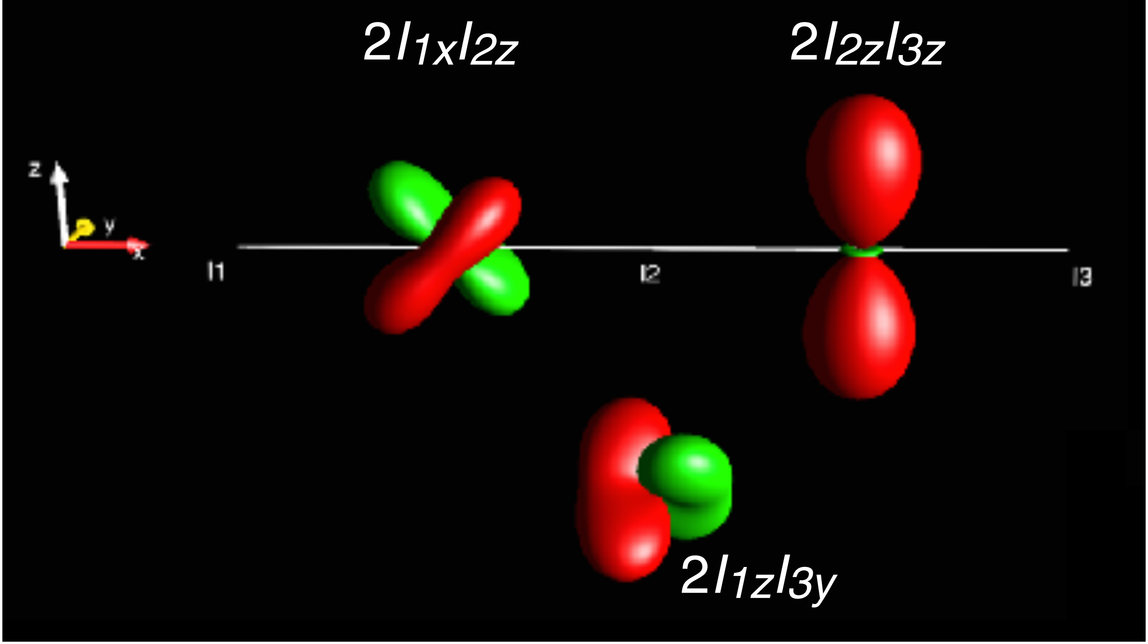
DROPS Display for a *Three-Spin Chain* (A)

For three-spin systems with $J_{13}=0$, the droplets representing *linear terms* can optionally be positioned on a line (rather than at the corners of a triangle) by selecting *Spin System > 3 Spin Chain*. The locations of the *bilinear terms*, of the *trilinear terms* and of the term proportional to the *identity operator* are schematically indicated below.

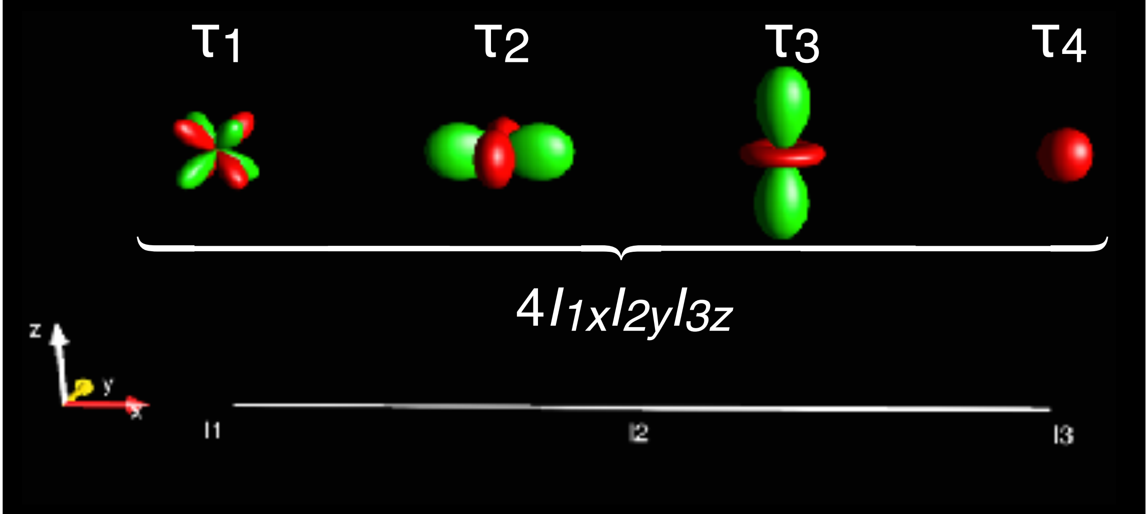


DROPS Display for a *Three-Spin Chain* (B)

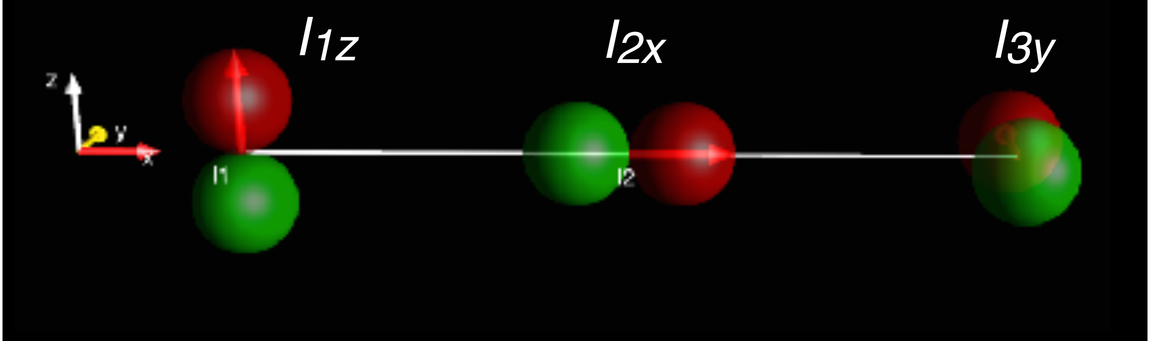
bilinear terms



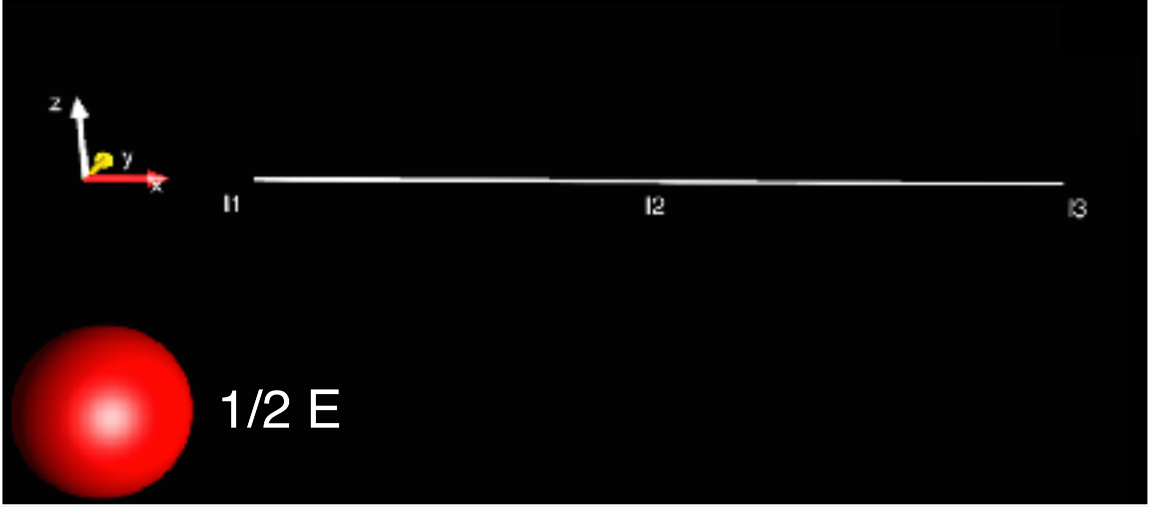
trilinear terms



linear terms

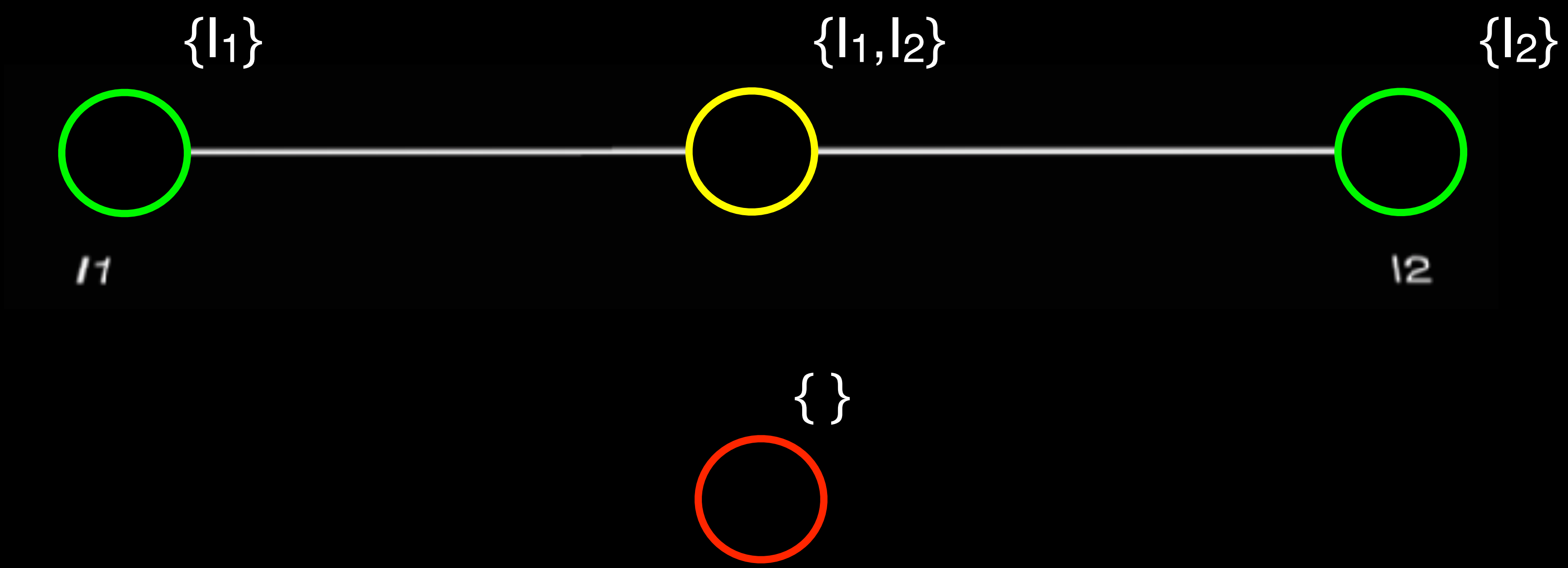


identity operator



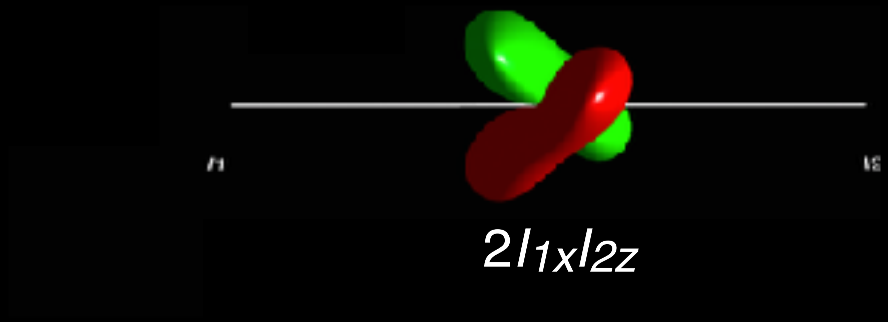
DROPS Display for *Two Spins* (A)

For systems consisting of two spins, the DROPS display can be adapted by selecting *Spin System > 2 Spins*. The locations of the *linear terms*, of the *bilinear term* and of the term proportional to the *identity operator* are schematically indicated below.

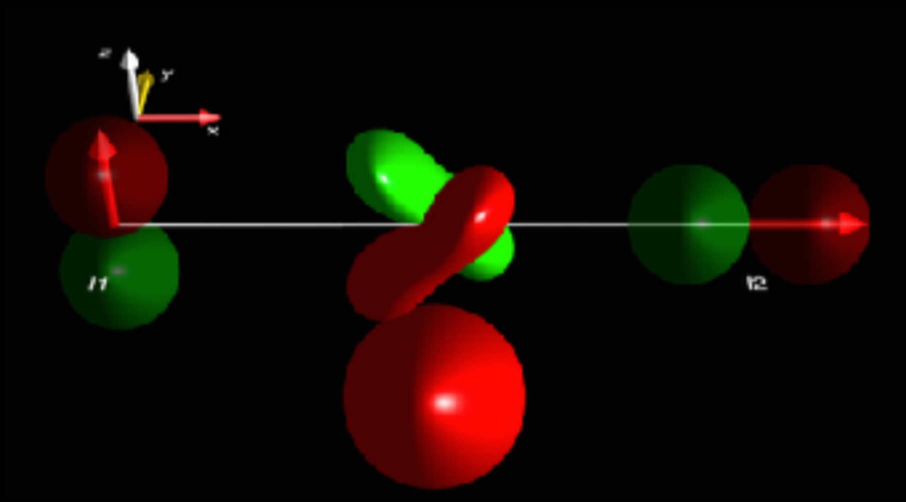


DROPS Display for *Two Spins* (B)

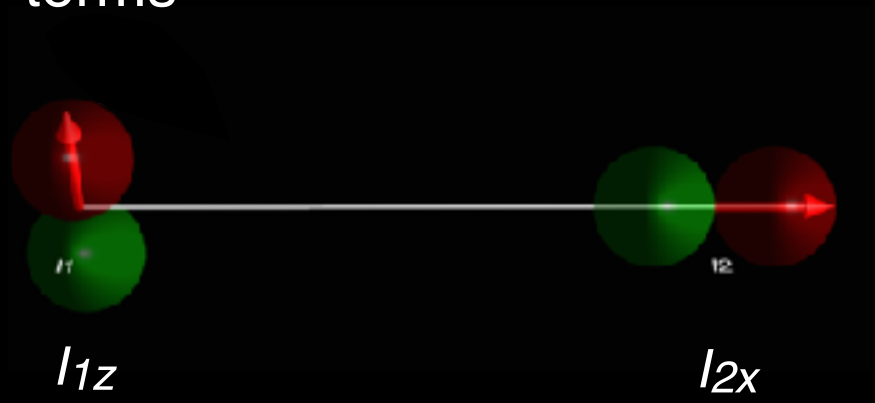
bilinear terms



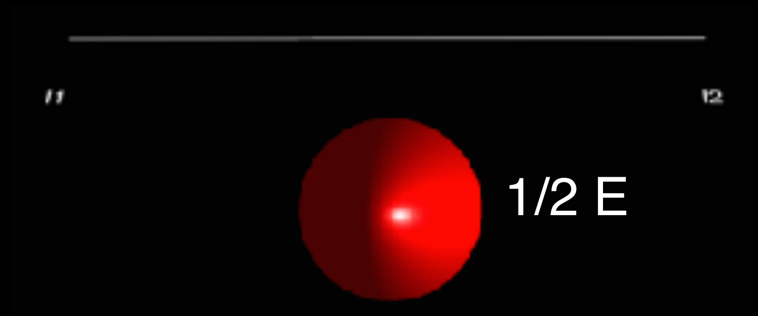
all terms



linear terms

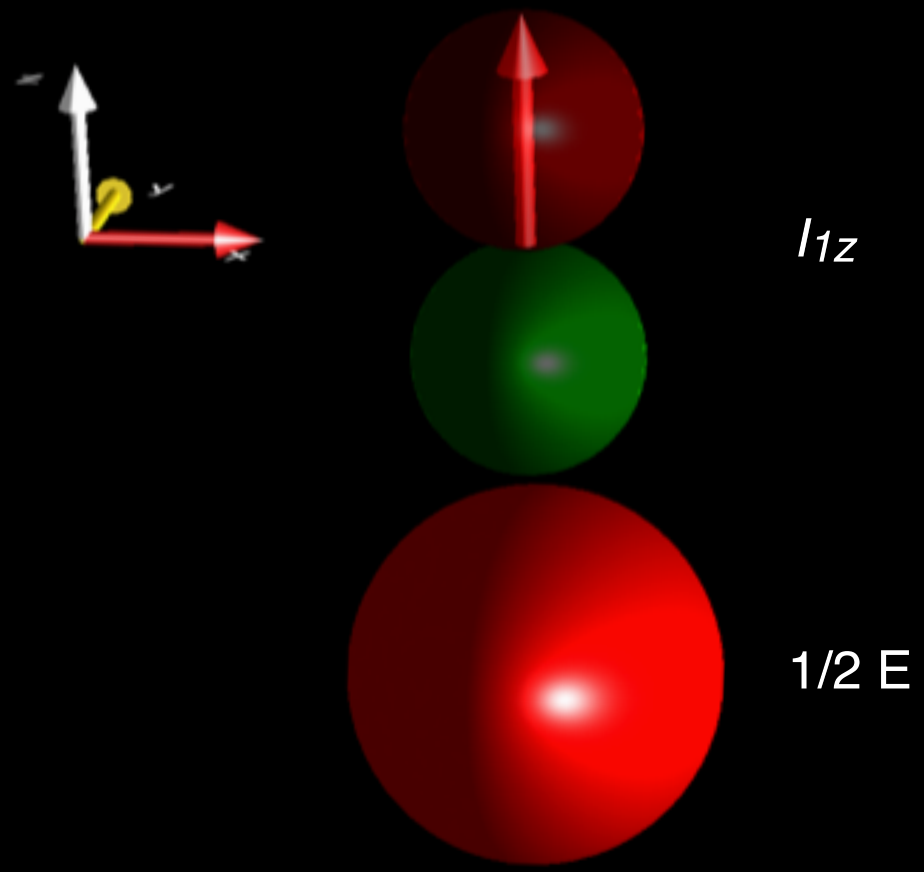


identity operator



DROPS Display for *a Single Spin*

For systems consisting of a single spin, the DROPS display can be adapted by selecting *Spin System* > 1 *Spin*. The term proportional to the *identity operator* is located below the *linear term*.



Display Options (A)

This menu allows you to choose the desired display options.

Selecting *List Prod. Ops.* displays a list of the current product operator terms. This list can be hidden by choosing *Display Options > Hide Prod. Ops.* (or by displaying a different list).

Selecting *List/Edit Seq.* displays the elements of the current pulse sequence and allows you to edit the sequence (for details, see *Help > Sequence Editor*). This list can be hidden by choosing *Display Options > Hide List Seq.* (or by displaying a different list).

The graphical display of the current pulse sequence can be switched off by selecting *Hide Seq. Plot*. It can be switched on again by selecting *Display Options > Show Seq. Plot*.

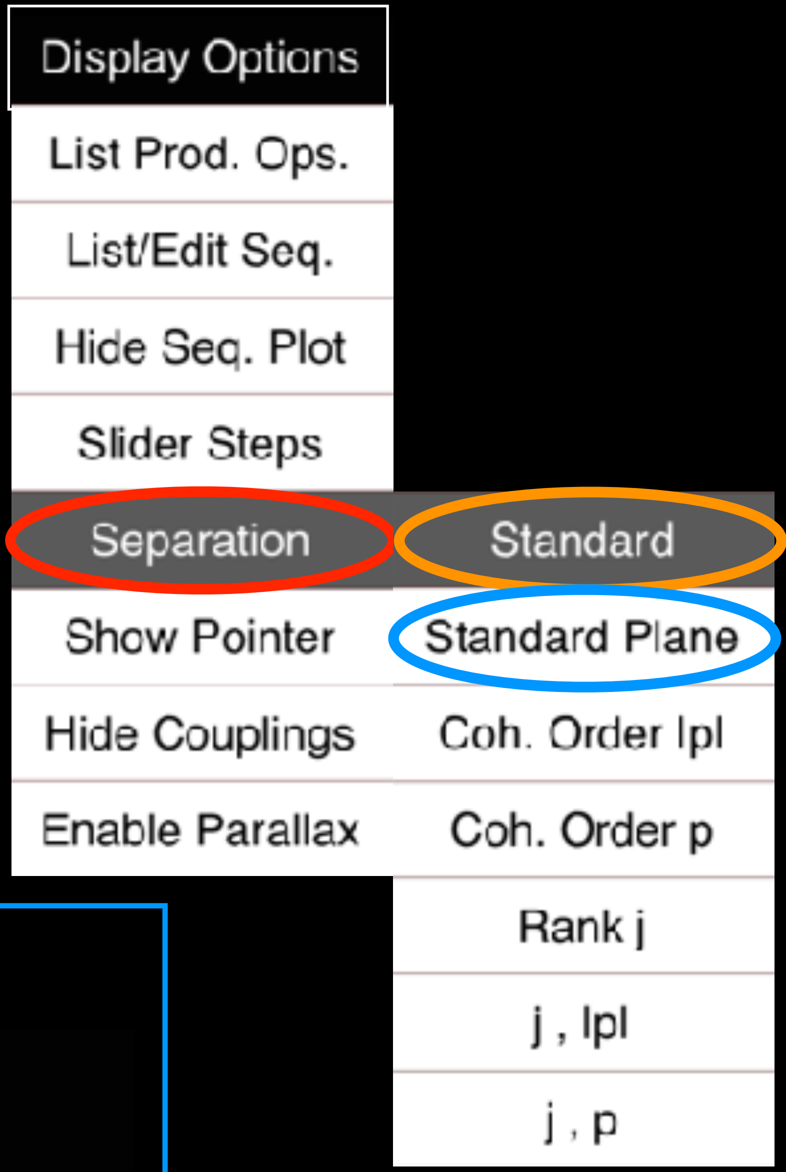
The button *Slider Steps* allows you to choose either "*Smooth*" or "*Discrete*" mode for the sliders to set the spin system parameters. In "*Smooth"* mode, the parameters can be adjusted continuously, whereas in "*Discrete*" mode, they are adjusted in steps of 0.1, which helps to set e.g. a given coupling constant to a value of exactly 0.0 or 1.0.

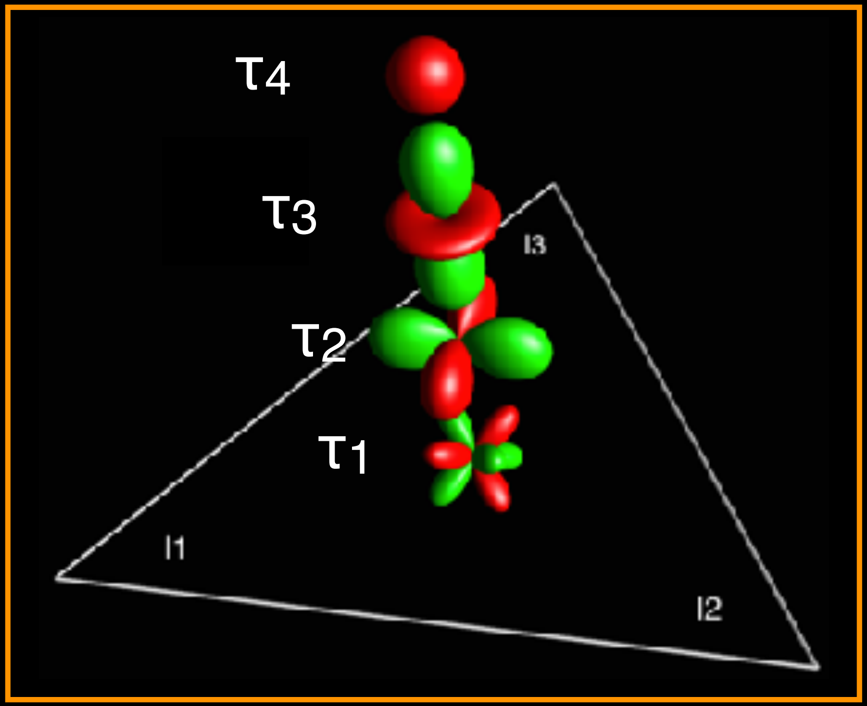
The option *Enable Parallax* allows you to interactively change the perspective of the DROPS display by simply tilting your device. This provides enhanced intuitive depth perception, which can be particularly helpful when looking at some of the more complex arrangements of droplets introduced in the following pages.

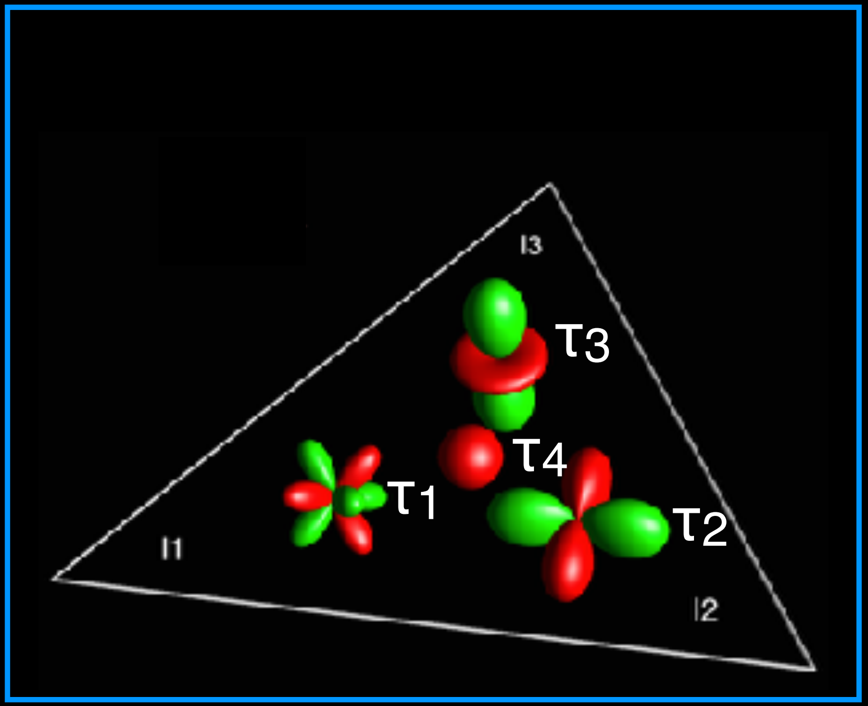
Display Options (B): Separation

The button *Separation* allows you to select one of several alternative advanced modes of the DROPS display in addition to the compact "*Standard* " DROPS display mode (c.f. *Help > Tutorial > DROPS Display*). In particular, it is possible to partition the compact standard droplets in terms of coherence order *p and/or* rank *j*.

In "*Standard Plane*" mode, the same droplets are shown as in "*Standard* " mode, but now all droplets - including the trilinear terms - are located in a single plane (in preparation for the other separation modes). In the example below, the operator $4I_{1x}I_{2y}I_{3z}$ is shown in "*Standard* " mode (left panel) and "*Standard Plane*" mode (right panel).





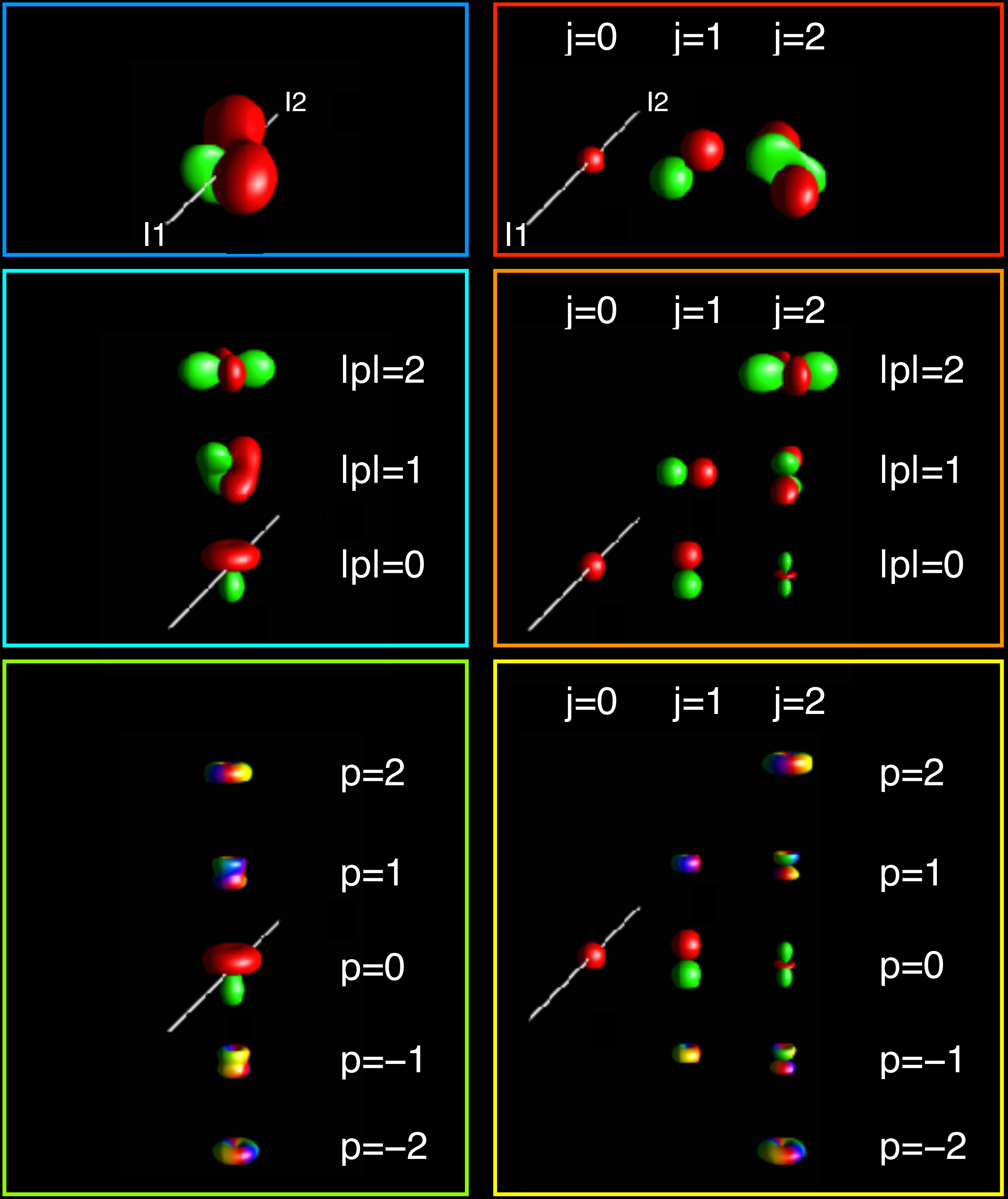


Display Options (C): Separation

To see the coherence orders and tensor ranks contained in a given state, the standard droplets can be split into sub droplets according to the following "*Separation*" options:

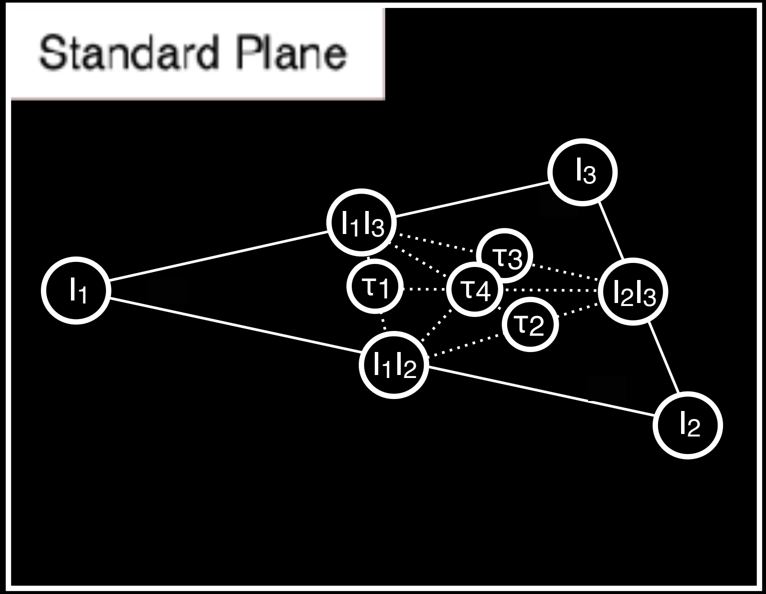
- absolute value of coh. order |*p*|,
- coherence order *p*,
- tensor rank *j*,
- *j* and |*p*|,
- *j* and *p*.

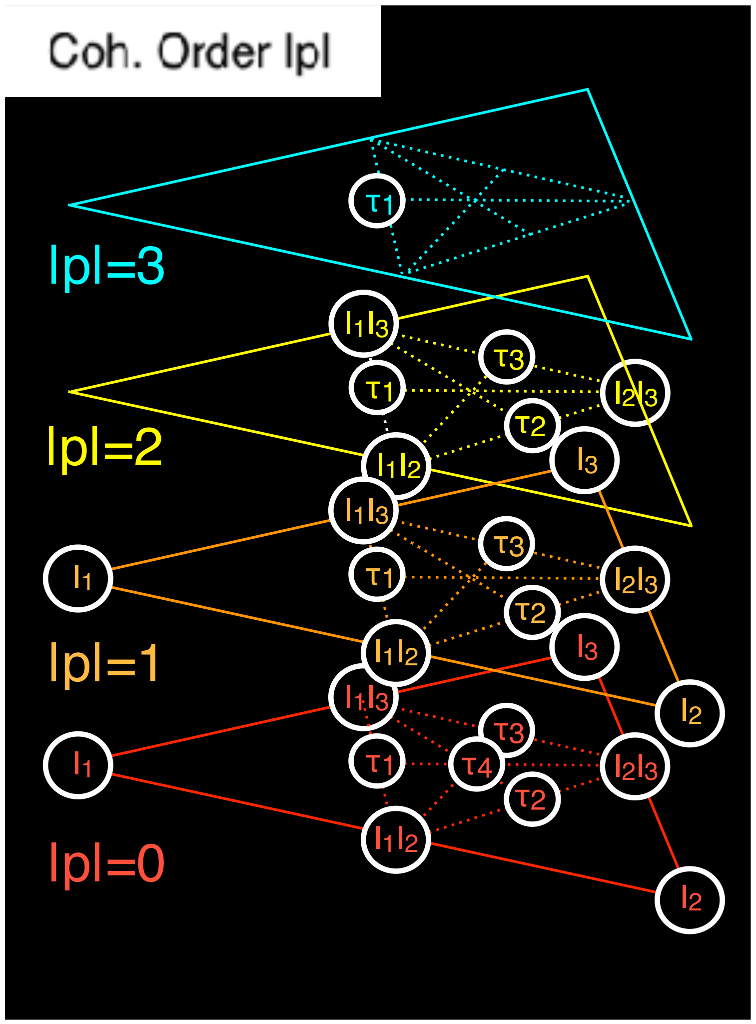
At the right, the different separation modes are illustrated for the example of the operator ($I_{1x}I_{2x} + I_{1x}I_{2y} + I_{1x}I_{2z}$).

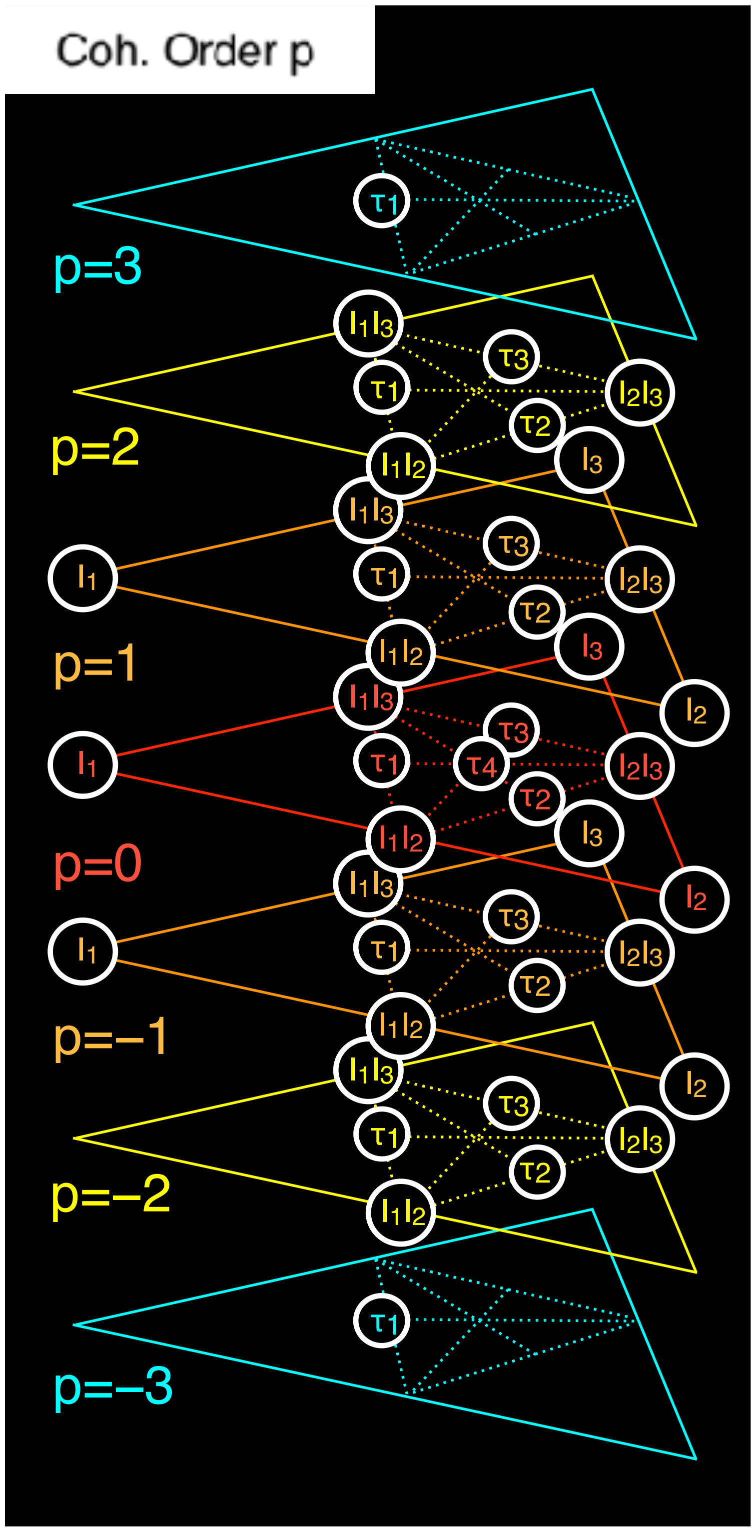


Display Options (D): Separation Based on Coherence Order

Schematic representation of droplet locations in a single plane (*Standard Plane*) or in multiple planes based on coherence order for a three-spin system.





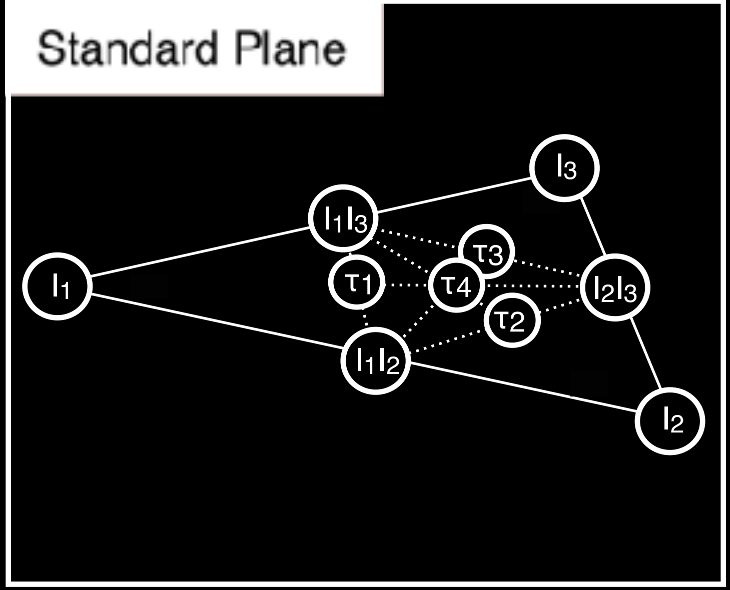


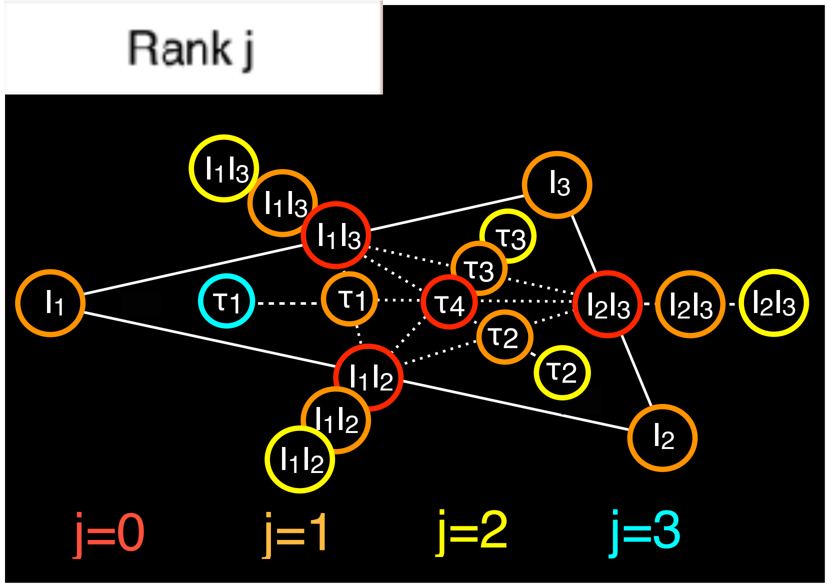
The planes and the droplet labels are color coded to indicate the different coherence levels: $p=0$ (red), $p=\pm1$ (orange), $p=\pm2$ (yellow), $p=\pm3$ (blue). For example, the linear operators represented by the droplet I_1 only contain coherence orders 0 and ±1. Only the trilinear operators represented by droplet τ_1 can have coherence orders p in the full range $-3 \le p \le 3$.

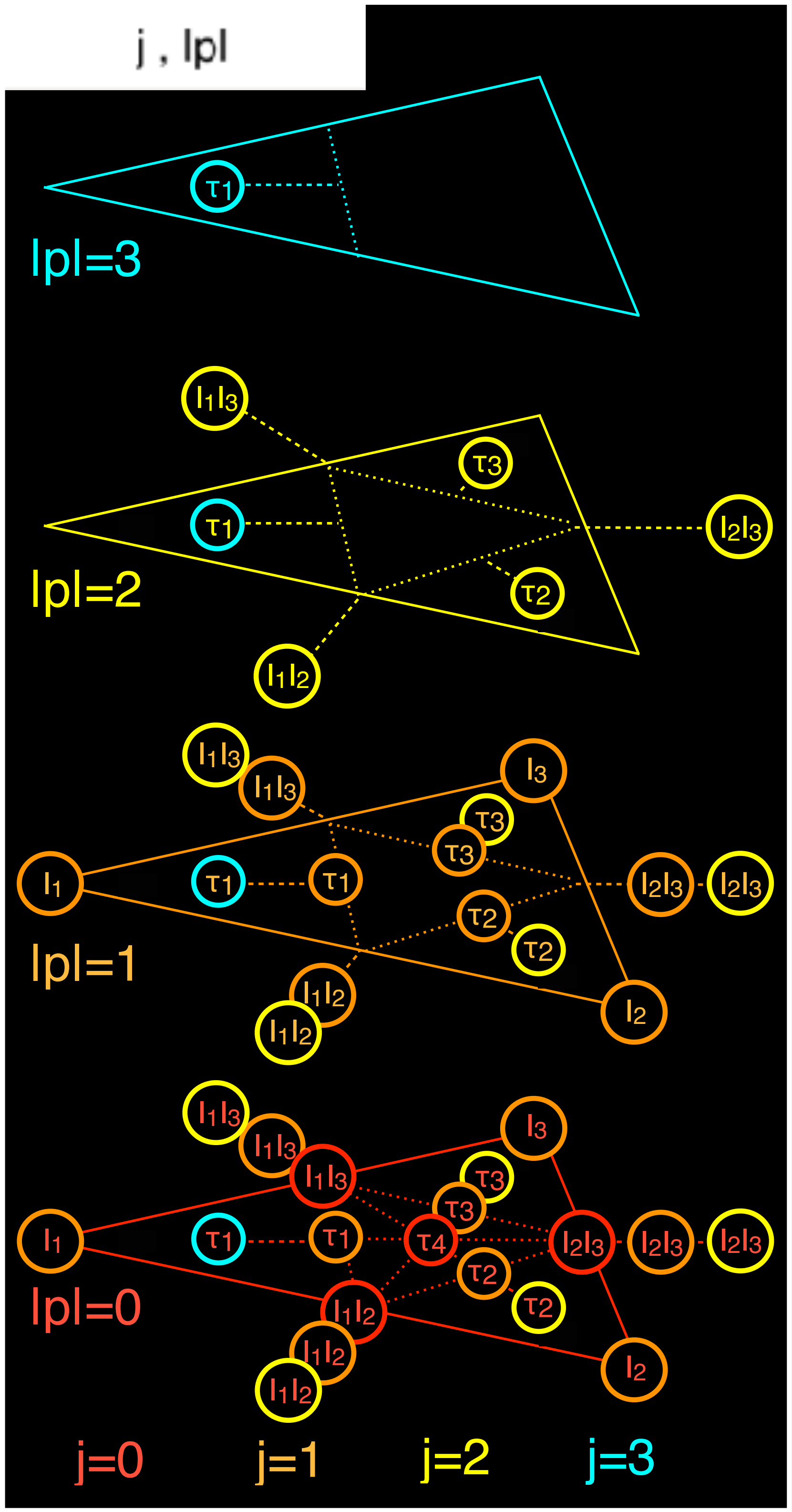
Display Options (E): Separation Based on Tensor Rank *j*

Schematic representation of the location of the droplets in the "*Standard Plane*" representation, in the "*Rank j*" display mode and in the "j, |p|" representation, where the standard droplets are split and separated based on both rank *j* and the absolute value $|p|$ of coherence order. (For more details on the rank of operators, see the section „Tensor grouping in the LISA basis" in *Help > Math > LISA Basis*). Here, the color of each circle indicates the rank *j* of the corresponding droplet and the color of the droplet label indicates the absolute value $|p|$ of its coherence order, which is limited to the range $0 \le |p| \le j$.

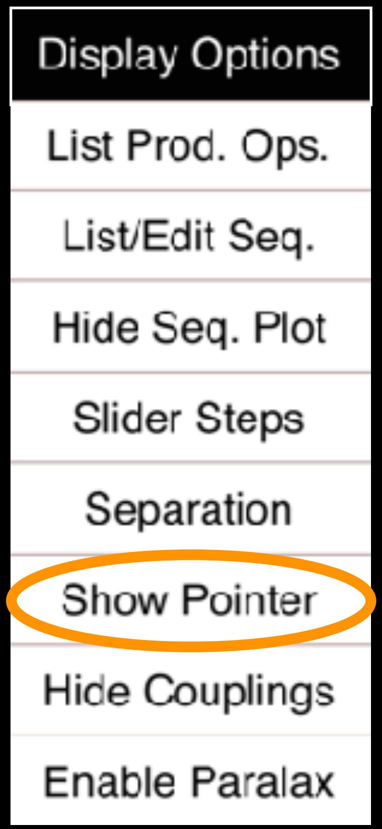
For example, the droplet "I_1I_2" representing bilinear operators involving spins I_1 and I_2 contains tensors of rank j=0 (red circle) with $|p|$=0, tensors with rank j=1 (orange circles) with $|p| \in \{0, 1\}$, and tensors with rank j=2 (yellow circles) with $|p| \in \{0, 1,2\}$.





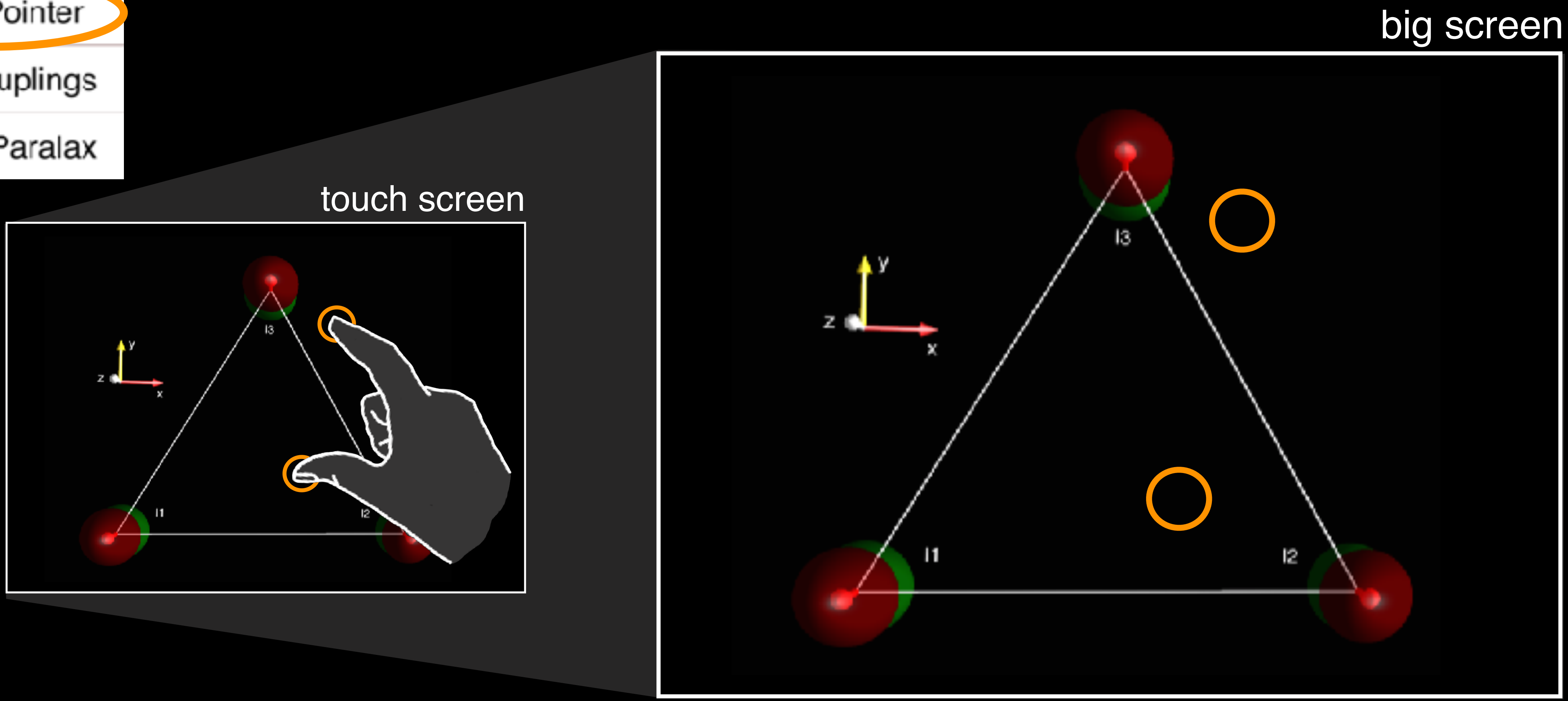


Display Options (F): Pointer



By choosing the option *Show Pointer*, touch points can be highlighted by orange circles.

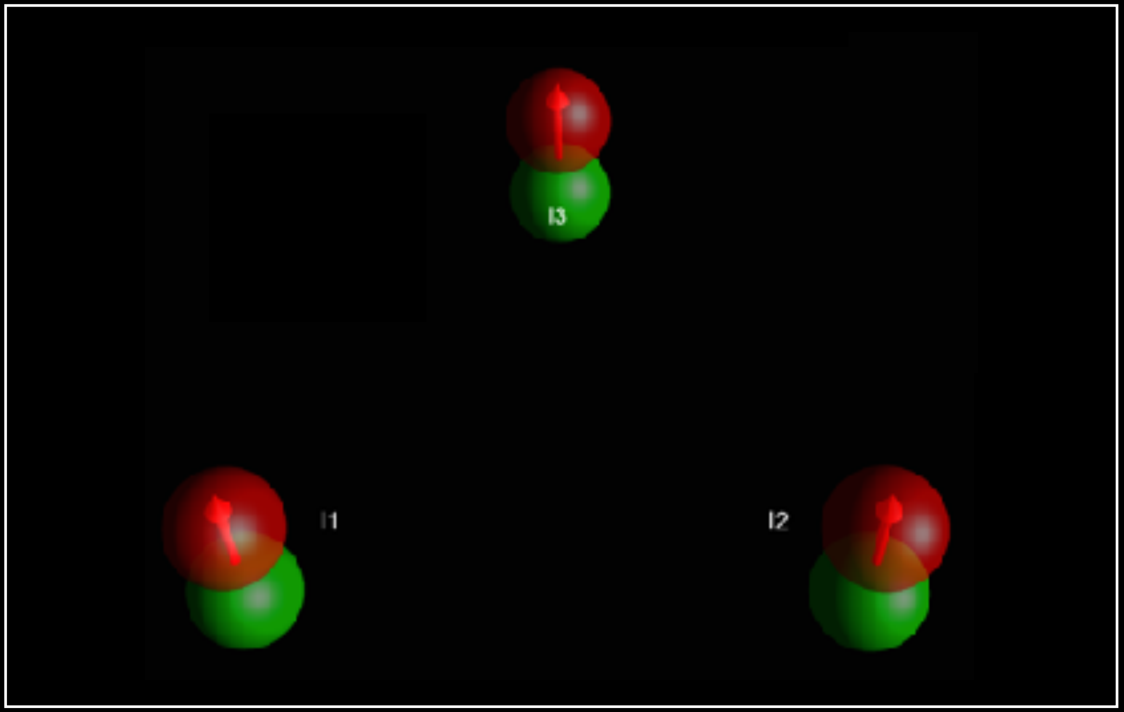
This option is particularly useful when the *SpinDrops* display is projected on a big screen. For example during a lecture, a touch point can be used as a pointer to focus attention on specific items on the screen. This option can also help to explain the effects of touch gestures when the position of the fingers cannot be seen on the big screen, see example below.

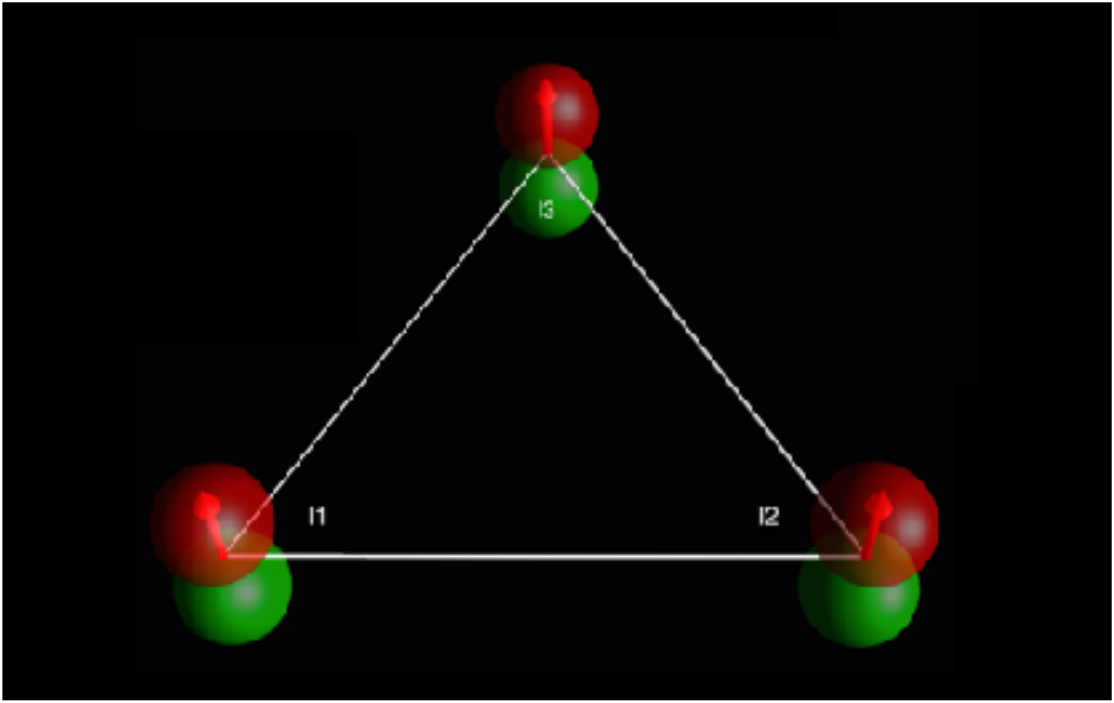


Display Options (G): Show/Hide Couplings

By default, the *J* couplings between spins are indicated by lines. To remove these lines, select *Hide Couplings*.

To show the lines again, select *Show Couplings*.

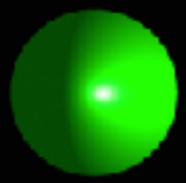
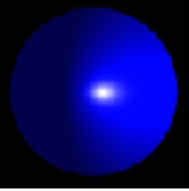




Color Code

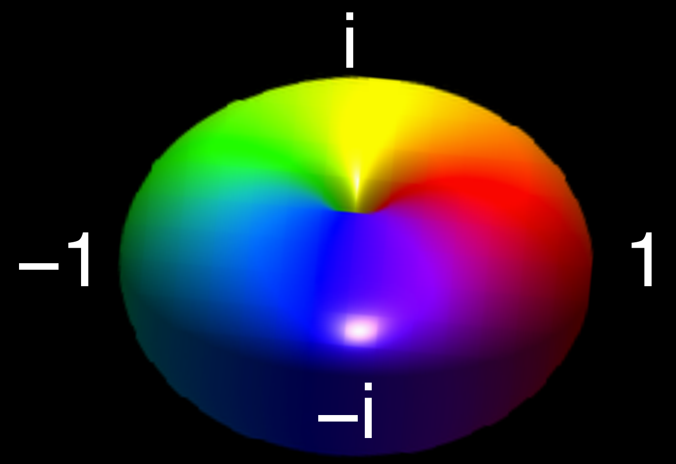
Color Code for Droplets (A)

Each *droplets* represents a complex function on a sphere (for more details, see *Help > Mathematical Background*). Any complex number c can be expressed in the form $c=r\exp(i\phi)$, where r is the *absolute value* (represented by the distance from the origin of a given droplet), ϕ is the *phase* and $\exp(i\phi)$ is the *phase factor* of the complex number (represented by the color wheel shown on the next page). The examples below show the colors of a spherical droplet with phase factors $\exp(i\phi)$ of 1 (red), i (yellow), –1 (green) and –i (blue).

ϕ[deg]	ϕ[rad]	$\exp(i\phi)$	Color	Droplet Example
0°	0	1	Red	
90°	$\pi/2$	i	Yellow	
180°	π	-1	Green	
270°	$3\pi/2$	$-i$	Blue	

Color Code for Droplets (B)

Color wheel representing phase factors $\exp(i\phi)$:



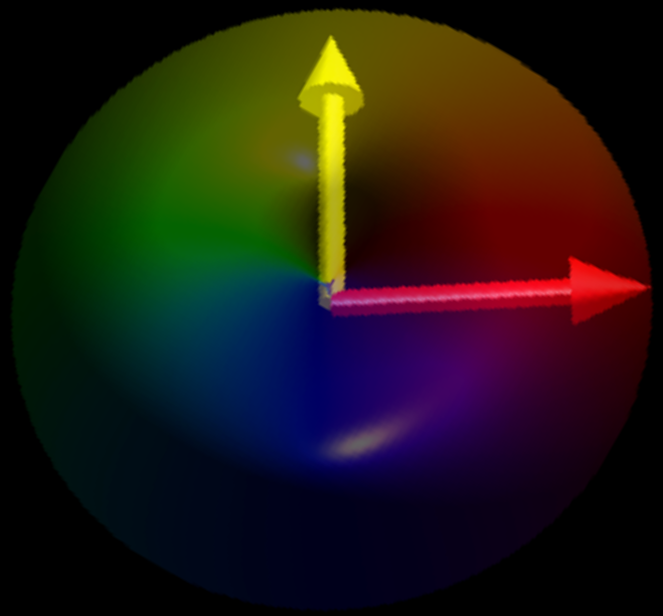
Note 1: This color wheel is slightly different from the one used in *Garon et al. (2015)*, where $\phi=\pi$ is cyan, rather than green. Opposing colors are used for phase factors with opposite signs: Red and green correspond to phase factors of 1 and –1, whereas yellow and blue correspond to the phase factors i and –i, respectively.

Note 2: We are aware of the relatively high prevalence of red-green color blindness and we are interested in evaluating optional alternative color wheels. Please contact us at drops@glasersystems.de if you are interested in evaluating such alternatives.

Color Code for Vectors

Linear Cartesian spin operators, such as I_{1x}, I_{1y} *or* I_{1z} are Hermitian and can always be represented as three-dimensional *real* vectors. If linear Cartesian spin operators are multiplied by i, the resulting operators i I_{1x}, i I_{1y} *or* i I_{1z} are skew-Hermitian, which can be represented by three-dimensional *imaginary* vectors.

Real vectors are represented by *red* arrows and imaginary vectors are represented by *yellow* arrows. This is illustrated below for the example of the raising operator $I_1^+ = I_{1x} + \mathrm{i}\, I_{1y}$, for which the term I_{1x} is represented by a real vector pointing along the x axis (red arrow) and the term i I_{1x} is represented by an imaginary vector pointing along the y axis (yellow arrow).



Color Code for Pulses

The following color code is used to represent the phase of a pulse in the graphical representation of a pulse sequence:

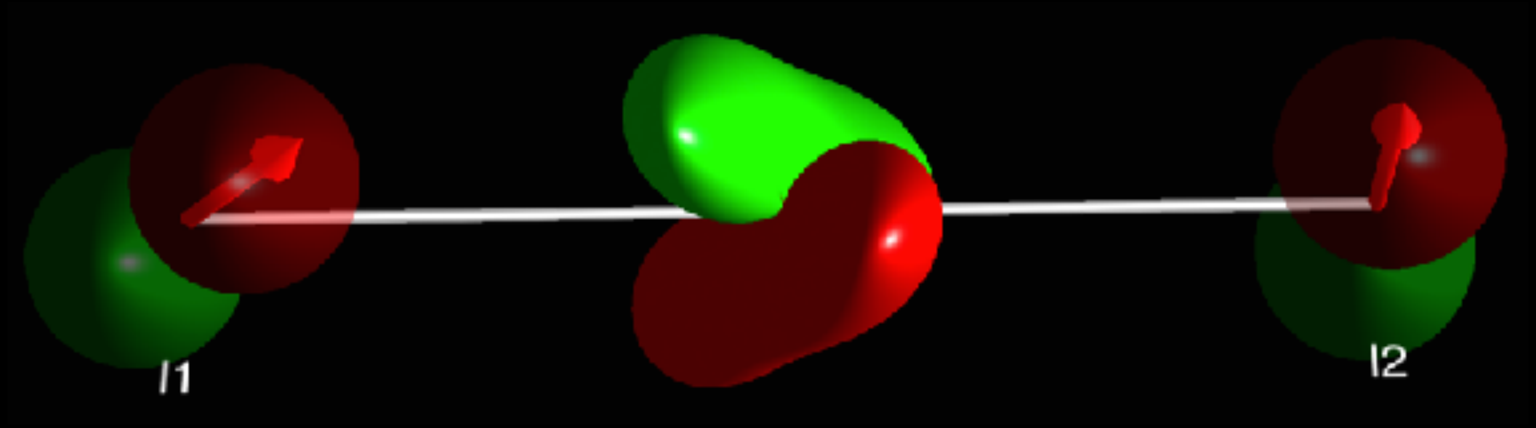
	Pulse Phase		Pulse Color	Pulse Example
[Cartesian]	[deg]	[rad]		
x	0°	0	Red	🟥
y	90°	π/2	Yellow	🟨
–x	180°	π	Green	🟩
–y	270°	3π/2	Blue	🟦

Rotations around the z axis and periods of isotropic mixing are indicated by grey rectangles.

Properties of the DROPS Representation

Beyond Vectors: The DROPS Representation of Operators

The states of uncoupled spins ½ can be completely described using three-dimensional Bloch vectors (commonly called “magnetization vectors” in NMR). However, in the general (and more interesting) case of coupled spins, the Bloch vector picture is not sufficient and more advanced concepts based on operators (such as product operators, density operators, Hamilton operators etc.) have to be used. While these operators and their time evolution can easily be calculated and manipulated by computer programs, they are difficult to visualize. In the **DROPS** representation, operators are displayed as a set of *droplets*, where each *droplet* corresponds to operators involving a defined set of spins (individual spins, pairs of spins, etc.).



To understand the general properties of the DROPS representation and to become familiar with the shapes of characteristic *droplets* requires a little practice, but is also fun, and highly rewarding. It not only provides a very intuitive visualization of spin dynamics. It is also extremely helpful to understand basic and advanced concepts of magnetic resonance spectroscopy (such as coherence order, phase cycles, polarization transfer etc.) that form the basis of modern pulse sequences design. In the following, we summarize and illustrate the most important properties of the DROPS display. For the mathematical background of the DROPS display, see *Help > Math*.

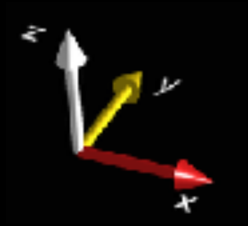
Droplets representing Linear Operators are Closely Related to the Vector Picture

For a *linear* Cartesian operator (i.e. operators such as I_{1x} or I_{1z} which involve only a single spin) the corresponding *droplet* consists of two spheres: a positive sphere (red) and a negative sphere (green). As illustrated on the right, the same is true for sums and differences of such operators (associated with the same spin, e.g. I_1) having real prefactors.

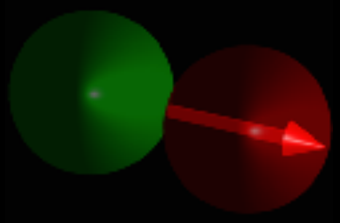
Such combinations of linear operators can also be represented as a single vector (the Bloch vector or magnetization vector in the case of the density operator).

An important property of the DROPS representation is that the Bloch vector is inscribed in the red sphere and the base of the vector touches the green sphere. Hence, the *orientation* of the droplet (defined as the direction of the vector connecting the centers of the green and red spheres) is always identical to the orientation of the corresponding Bloch vector.

For a single spin, the DROPS representation is closely related to the well-known vector picture. Therefore, a droplet representing the *linear* operators associated with a given spin is shown in transparent mode and the corresponding vector is shown simultaneously.

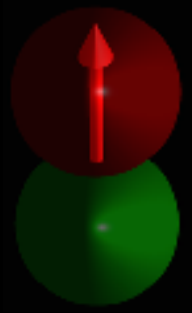


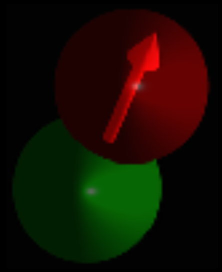
I_{1x}



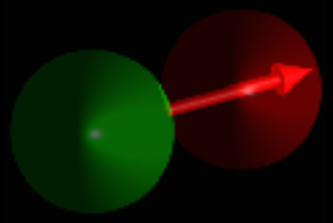
I_{1y}

I_{1z}





$0.3\ I_{1x} + 0.9\ I_{1z}$



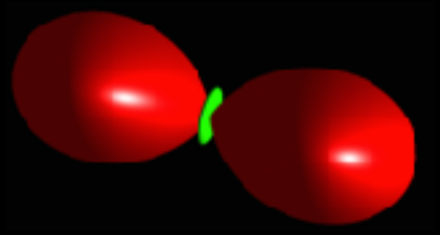
$0.7\ I_{1x} + 0.7\ I_{1y}$

Droplets of Cartesian Product Operators Are Real-Valued

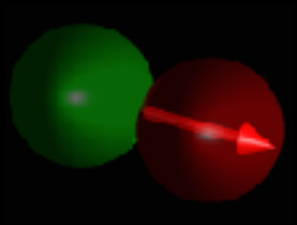
Droplets representing standard *Cartesian product operators* are real and thus can have only the colors *red* (for positive values) and/or green (for negative values). The standard color code of the droplets is explained in *Help > Color Code > Droplets*.

Examples of individual Cartesian product operators involving 0 spins (term proportional to the identity operator E), a single spin (linear operator) and two spins (bilinear operator) are shown below.

1/2 E

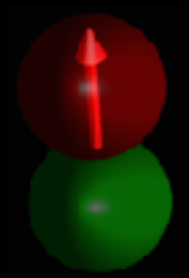


$2I_{1x}I_{2x}$

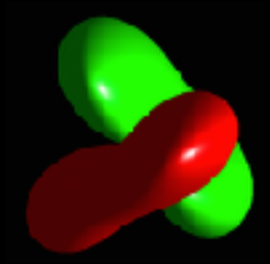


I_{1x}

$2I_{1x}I_{2y}$



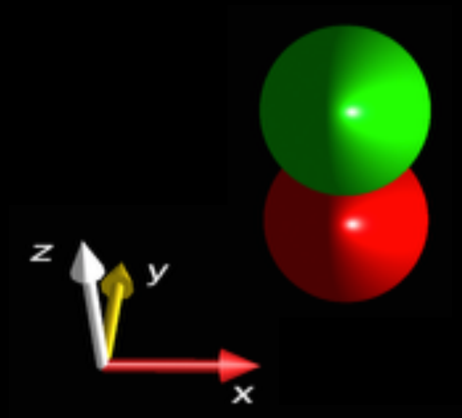
I_{1z}



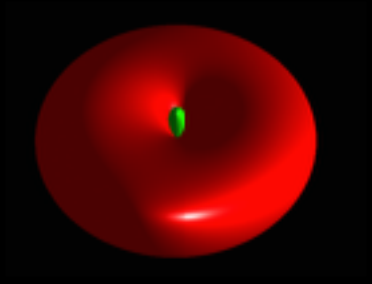
$2I_{1x}I_{2z}$

Droplets of Hermitian Operators Are Red/Green

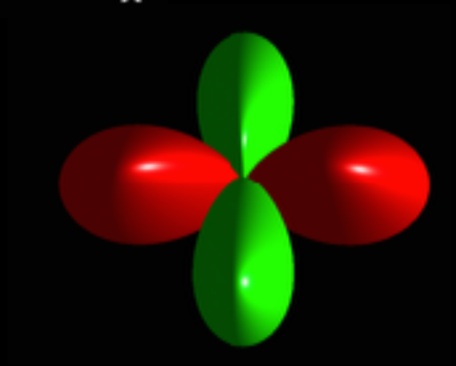
Droplets representing Hermitian operators (corresponding to *real* combinations of Cartesian product operators) can easily be recognized because they can only have the colors *red* or *green* or both.
Examples of some droplets representing Hermitian operators are shown below.



$2I_{1y}I_{2x} – 2I_{1x}I_{2y}$

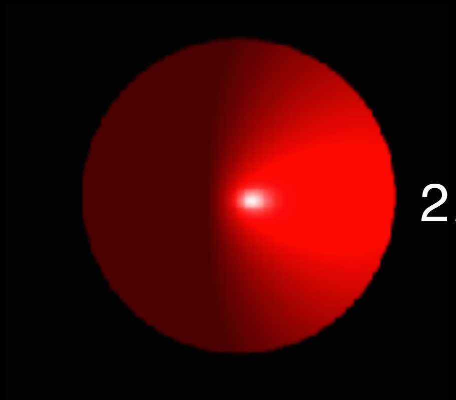


$2I_{1x}I_{2x} + 2I_{1y}I_{2y}$

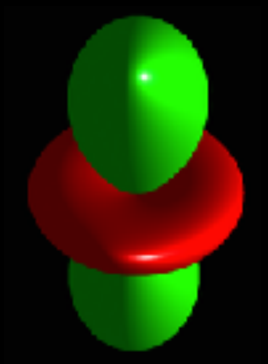


$2I_{1x}I_{2x} – 2I_{1y}I_{2y}$

$2I_{1x}I_{2y} + 2I_{1y}I_{2x}$



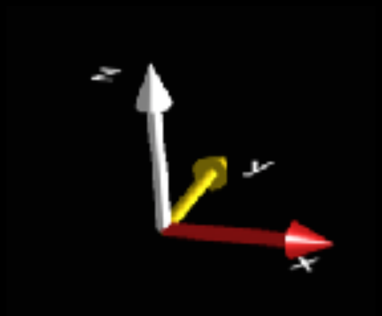
$2I_{1x}I_{2x} + 2I_{1y}I_{2y} + 2I_{1z}I_{2z}$

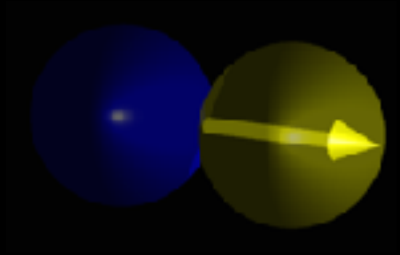


$I_{1x}I_{2x} + I_{1y}I_{2y} - 2I_{1z}I_{2z}$

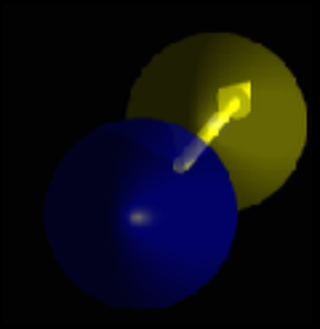
Droplets of Skew-Hermitian Operators Are Yellow/Blue

Multiplying Hermitian operator by the imaginary unit i results in so-called skew-Hermitian operators. The corresponding droplet functions are purely imaginary. Their droplets can only have the colors *yellow* (if the imaginary part of the droplet function is positive) or *blue* (if the imaginary part of the droplet function is negative). Examples of some droplets representing skew-Hermitian operators are shown below.



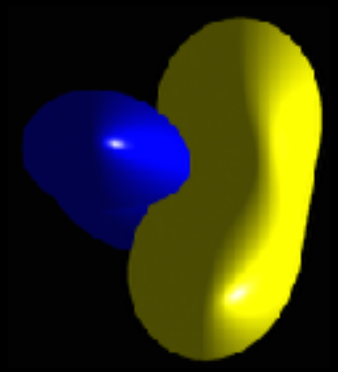


i I_{1x}



i I_{1y}

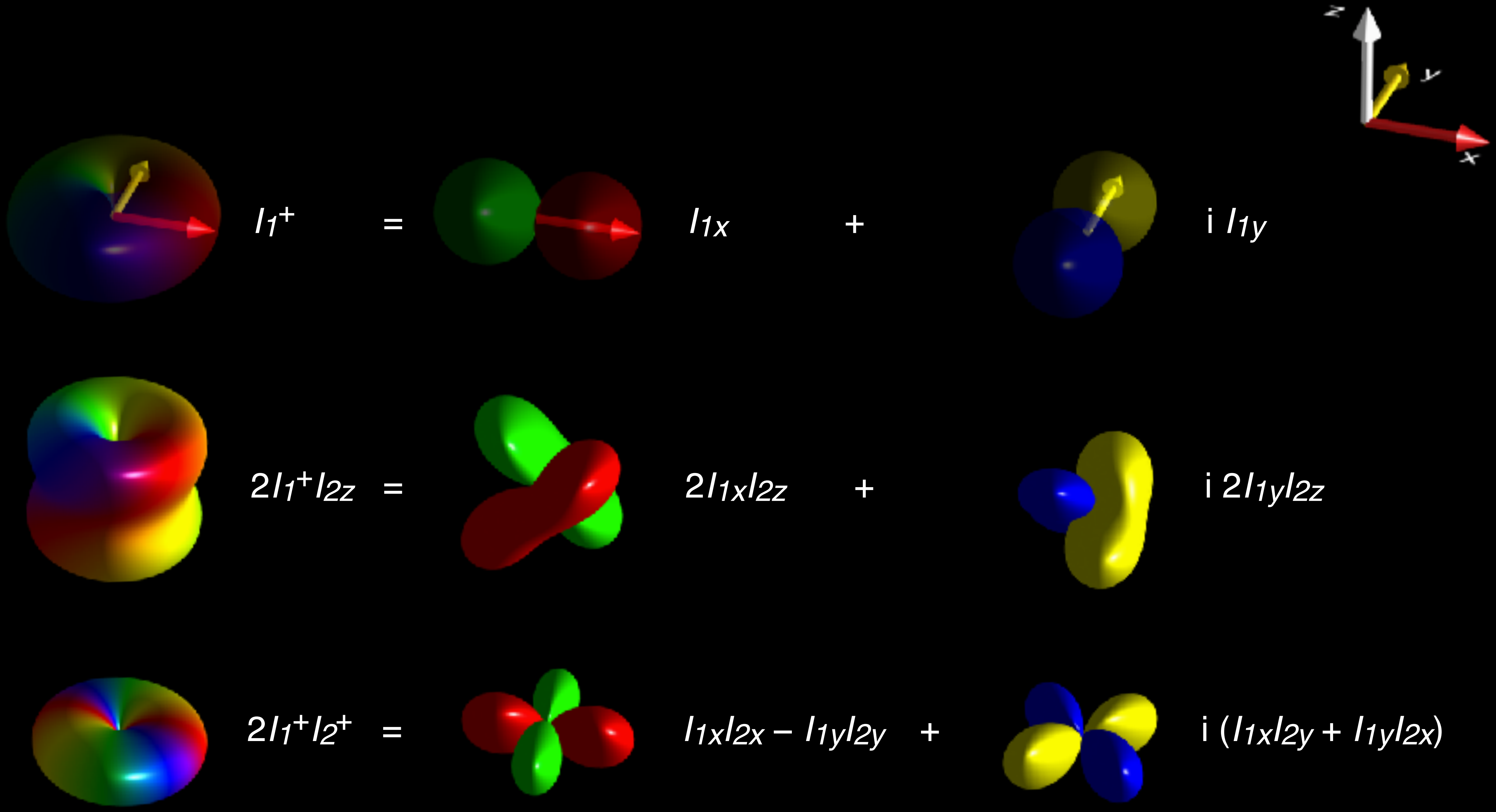
i $2I_{1x}I_{2z}$



i $2I_{1y}I_{2z}$

Droplets of Operators Consisting of Hermitian and Skew-Hermitian Components

Here we present important examples of operators which are neither purely Hermitian nor purely skew-Hermitian, i.e. they can be decomposed into Hermitian and skew-Hermitian parts:



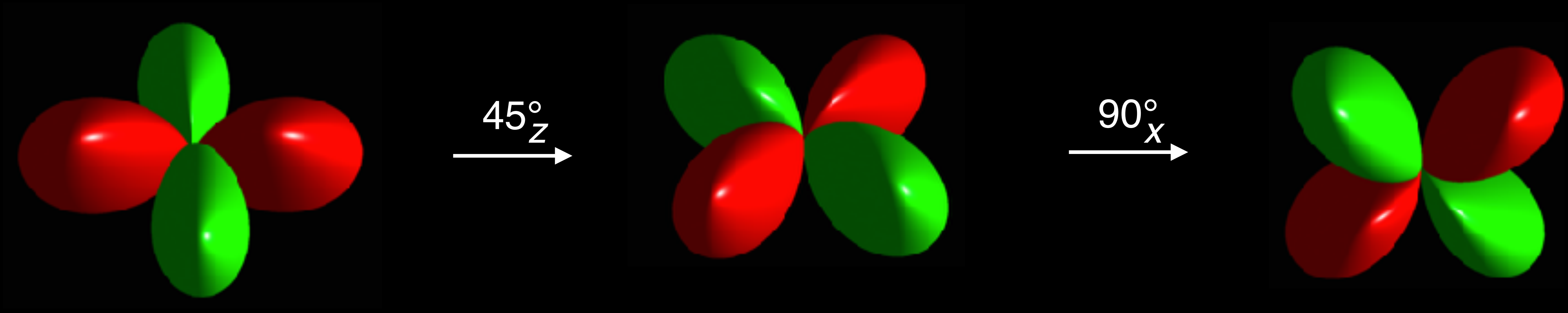
$I_1^+ = I_{1x} + i\, I_{1y}$

$2I_1^+I_{2z} = 2I_{1x}I_{2z} + i\, 2I_{1y}I_{2z}$

$2I_1^+I_2^+ = I_{1x}I_{2x} - I_{1y}I_{2y} + i\, (I_{1x}I_{2y} + I_{1y}I_{2x})$

Non-Selective Rotations of Operators Simply Rotate the Droplets

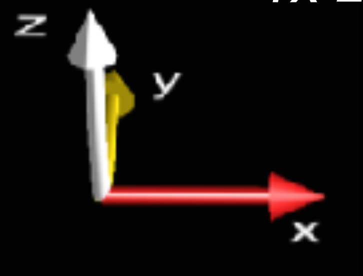
Rotating an operator by a given angle about a given axis also rotates the corresponding droplets by the same angle about the same axis. This is one of the most important features of the DROPS representation. For example, rotating the operator $2I_{1x}I_{2x} - 2I_{1y}I_{2y}$ by 45° about the z axis results in $2I_{1y}I_{2x} + 2I_{1x}I_{2y}$ and an additional rotation by 90° about the x axis results in $2I_{1z}I_{2x} + 2I_{1x}I_{2z}$. Note that it is much more intuitive to recognize rotations based on the initial and final DROPS representations rather than based on the initial and final product operators.



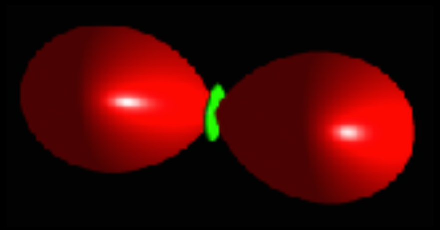
$2I_{1x}I_{2x} - 2I_{1y}I_{2y}$

$2I_{1y}I_{2x} + 2I_{1x}I_{2y}$

$2I_{1z}I_{2x} + 2I_{1x}I_{2z}$

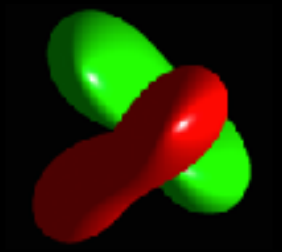


Characteristic Droplets of Cartesian Product Operators Involving Two Spins

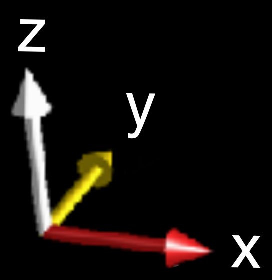


$2I_{1x}I_{2x}$

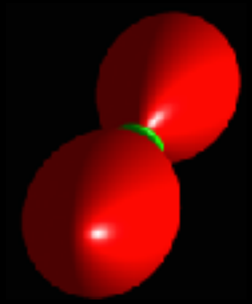
$2I_{1x}I_{2y}$



$2I_{1x}I_{2z}$



$2I_{1y}I_{2x}$

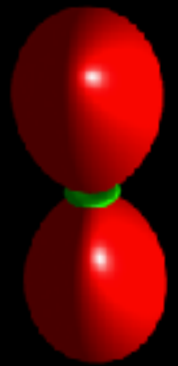


$2I_{1y}I_{2y}$

$2I_{1y}I_{2z}$

$2I_{1z}I_{2x}$

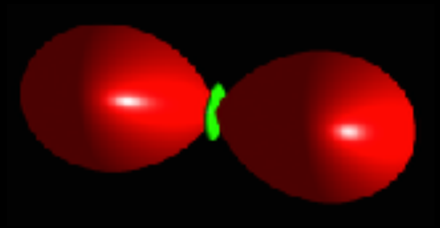
$2I_{1z}I_{2y}$



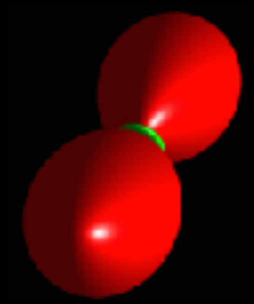
$2I_{1z}I_{2z}$

Droplets of Cartesian Product Operators of the Form $2I_{1a}I_{2a}$

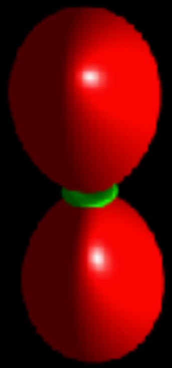
As shown on the previous page, the bilinear product operators $2I_{1x}I_{2x}$, $2I_{1y}I_{2y}$, and $2I_{1z}I_{2z}$ of the general form $2I_{1a}I_{2a}$ with $a \in \{x, y, z\}$ have elongated shapes along the a axis and can easily be recognized. They consist of two red (positive) lobes (oriented in the direction of a and $-a$, respectively) and a small green (negative) toroidal shape around the a axis.



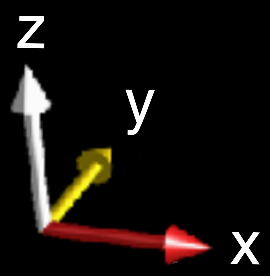
$2I_{1x}I_{2x}$



$2I_{1y}I_{2y}$



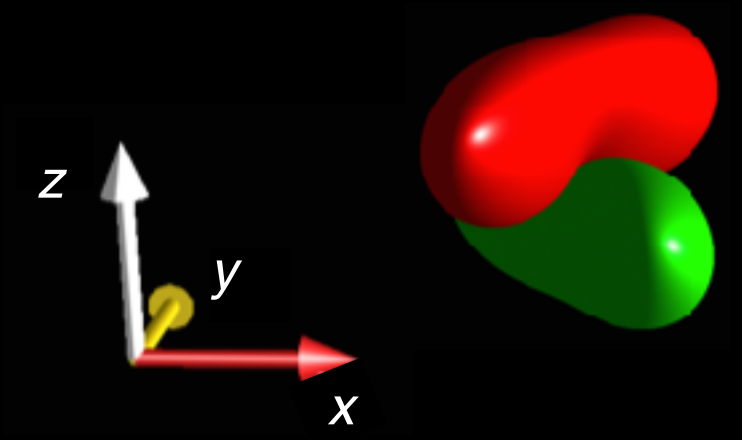
$2I_{1z}I_{2z}$



Droplets of Cartesian Product Operators of the Form $2I_{1a}I_{2b}$ (A)

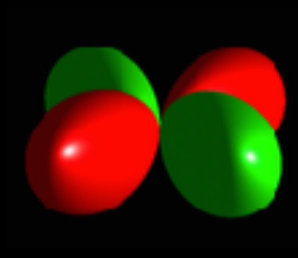
The operators $2I_{1a}I_{2b}$ with $a \neq b$ and $a, b \in \{x, y, z\}$ are represented by a droplet with *two bean-shaped lobes* of opposite signs, i.e. a red (positive) lobe and a green (negative) lobe. As all operators can be obtained by non-selective 90° rotations e.g. from $2I_{1x}I_{2y}$ (see *Challenge* 8 in *Help > Challenges*), here we focus on this operator to understand the origin of the characteristic shape of these droplets. Note that $2I_{1x}I_{2y}$ can be expressed as a linear combination of the double-quantum operator $\mathrm{DQ_y} = I_{1x}I_{2y}+I_{1y}I_{2x}$ (symmetric with respect to an exchange of the two spins) and the zero-quantum operator $\mathrm{ZQ_y} = -I_{1x}I_{2y}+I_{1y}I_{2x}$ (anti-symmetric with respect to an exchange of the two spins):

$$2I_{1x}I_{2y} = \mathrm{DQ_y} - \mathrm{ZQ_y} = \mathrm{DQ_y} + (-\mathrm{ZQ_y}) = (I_{1x}I_{2y}+I_{1y}I_{2x}) + (I_{1x}I_{2y}-I_{1y}I_{2x})$$



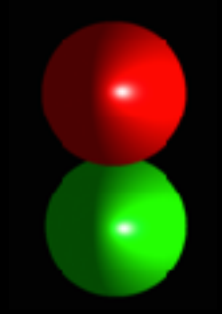
$2I_{1x}I_{2y}$

=



$\mathrm{DQ}_y = I_{1x}I_{2y} + I_{1y}I_{2x}$

+

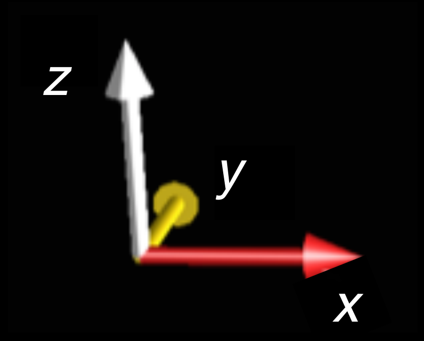


$-\mathrm{ZQ}_y = I_{1x}I_{2y} - I_{1y}I_{2x}$

Droplets of Cartesian Product Operators of the Form $2I_{1a}I_{2b}$ (B)

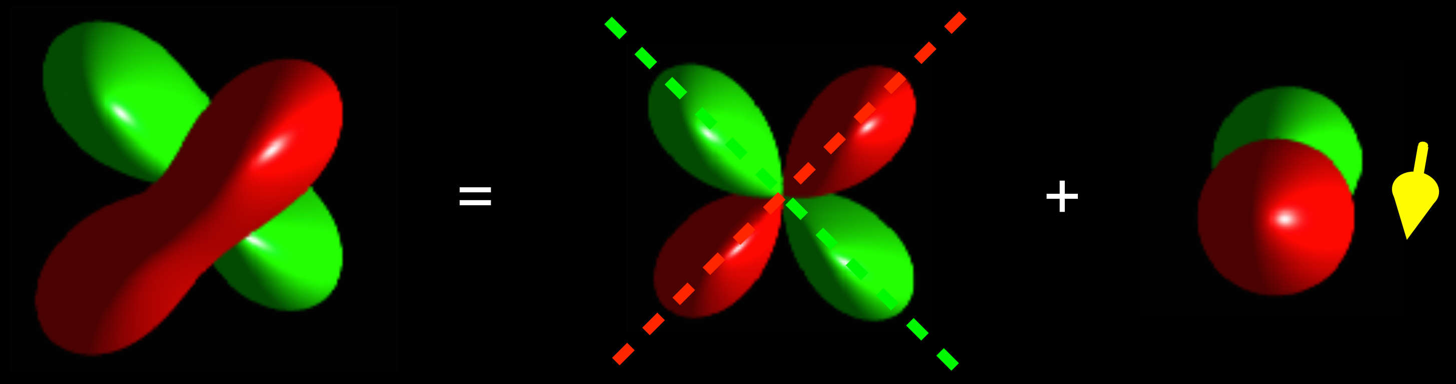
Similar to $2I_{1x}I_{2y}$, the antiphase operator $2I_{1x}I_{2z}$ can be expressed as a sum of a symmetric and an anti-symmetric term:

$2I_{1x}I_{2z}$ $\quad$ $I_{1x}I_{2z} + I_{1z}I_{2x}$ $\quad$ $I_{1x}I_{2z} - I_{1z}I_{2x}$

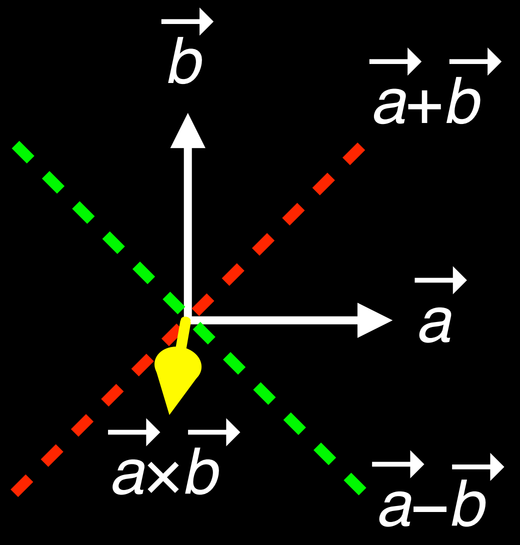


Droplets of Cartesian Product Operators of the Form $2I_{1a}I_{2b}$ (C)

In general, an operator $2I_{1a}I_{2b}$, where $a \neq b$ and $a, b \in \{x, y, z\}$, can always be written as a sum of the form $2I_{1a}I_{2b} = (I_{1a}I_{2b}+I_{1a}I_{2b}) + (I_{1a}I_{2b}-I_{1a}I_{2b})$. The droplet corresponding to the symmetric term in the first bracket is “X-shaped” and consists of two red (positive) lobes oriented along the *axis* of the vector sum $\vec{a}+\vec{b}$ (dashed red line) and two green (negative) lobes oriented along the *axis* of the vector difference $\vec{\mathrm{a}}-\vec{\mathrm{b}}$ (dashed green line). The droplet corresponding to the anti-symmetric term in the second bracket consists of a red (positive) and a green (negative) sphere, where the red sphere is displaced relative to the green sphere in the direction given by the cross product $\vec{a}\times\vec{b}$ (yellow arrow). In the DROPS representation of $2I_{1a}I_{2b}$, the red (and green) lobes of $(I_{1a}I_{2b}+I_{1a}I_{2b})$ and $(I_{1a}I_{2b}-I_{1a}I_{2b})$ merge, forming the characteristic droplet consisting of a red and green bean-shaped lobe.



$2I_{1a}I_{2b}$ $\qquad$ $I_{1a}I_{2b} + I_{1b}I_{2a}$ $\qquad$ $I_{1a}I_{2b} - I_{1b}I_{2a}$



Droplets of Cartesian Product Operators of the Form $2I_{1a}I_{2b}$ (D)

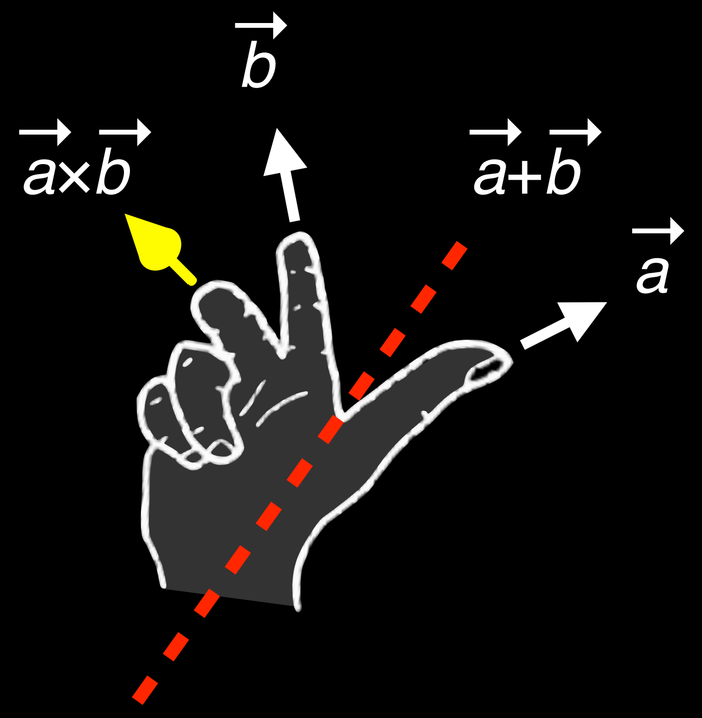
Right-hand rule

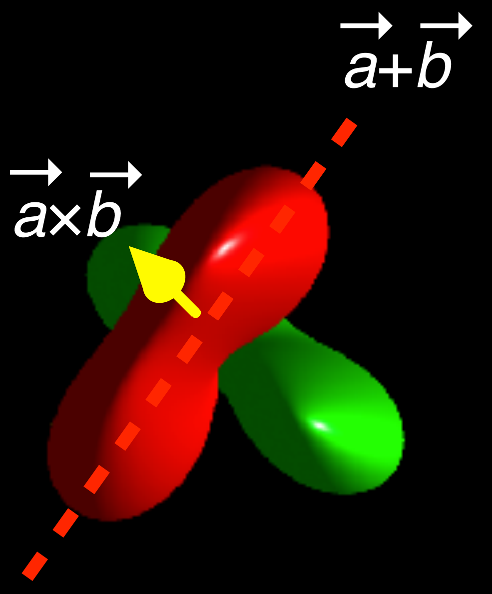
The shape and color of the droplet representing a Cartesian product operators of the form $2I_{1a}I_{2b}$, where $a \neq b$ and a, $b \in \{x, y, z\}$, can be constructed and analyzed using the following *right-hand rule*:

(a) Point the thumb of your right hand in the direction of the unit vector $\vec{a}$ and the index finger in the direction of $\vec{b}$.

(b) The bisector of the angle formed by the thumb and index finger defines the *axis* of the vector sum $\vec{a}+\vec{b}$ (dashed red line). This defines the long axis of the bean-shaped *red* lobe of the droplet. (Orthogonal to the red axis, the long axis of the *green* bean-shaped lobe is oriented along the axis defined by $\vec{a}-\vec{b}$.)

(c) Relative to the center of the droplet, the *red* lobe is displaced in the direction given by the cross product $\vec{a}\times\vec{b}$ (yellow arrow), which is given by the orientation of the middle finger of your right hand. (The *green* lobe is displaced in the opposite direction.)





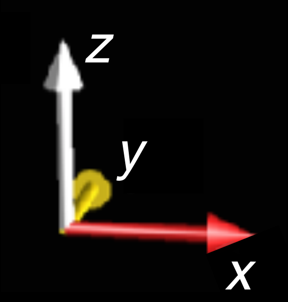
$2I_{1a}I_{2b}$

Droplets of Antiphase Operators, Kissing Beans (A)

Based on the rules summarized on the previous page, a given *droplet* of an antiphase operator can be translated back into the form of a product operator (see *Help > Challenges*). As illustrated below, it is even simpler to recognize which of the involved two single spin operators is a *z* operator, i.e. to determine if the coherence is in antiphase with respect to the first or the second spin. Imagine the red and green lobes to be a pair of “kissing beans”. If the “heads” of the kissing beans are tilted to the *left* (relative to the *z* axis), the component of the *first* spin operator is *z* and the component of the *second* spin is in the transverse plane (i.e. the antiphase operator has the form $\pm 2I_{1z}I_{2a}$ with $a \in \{x,y\}$). Conversely, if the “heads” are tilted to the *right*, the *second* single spin operator is a *z* operator and the Cartesian component of the *first* spin is in the transverse plane ($\pm 2I_{1z}I_{2a}$). In the general case of operators involving spins I_m and I_n with $m<n$, a tilt to the *left* indicates that the I_m operator is a *z* operator and vice versa.

Left tilt:

Right tilt:



Droplets of Antiphase Operators, Kissing Beans (B)

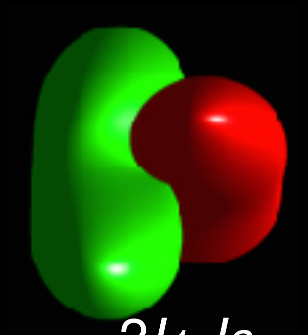
Here, the “head-tilt rule” is shown for all antiphase operators involving spins I_1 and I_2.

Left tilt: Antiphase coherence of spin I_2 with respect to spin I_1

$2I_{1z}I_{2x}$

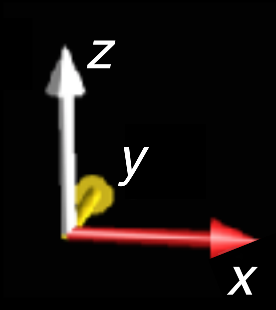
$2I_{1z}I_{2y}$

$-2I_{1z}I_{2x}$

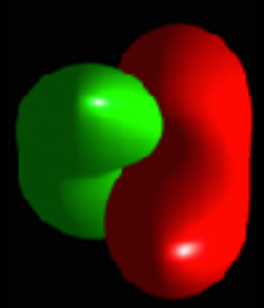


$-2I_{1z}I_{2y}$

Right tilt: Antiphase coherence of spin I_1 with respect to spin I_2



$2I_{1x}I_{2z}$



$2I_{1y}I_{2z}$

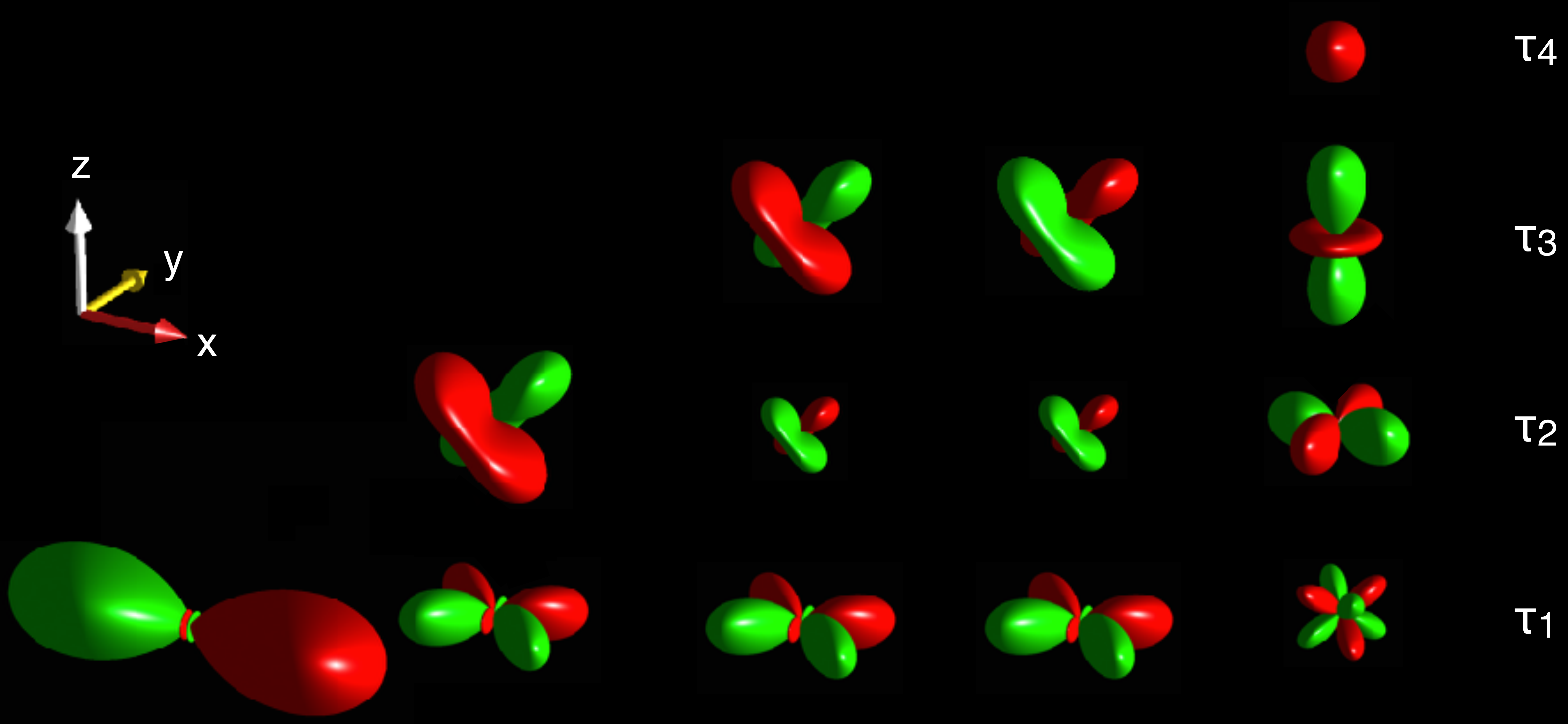
$-2I_{1x}I_{2z}$

$-2I_{1y}I_{2z}$

(By the way, an interesting study of human head-turning asymmetry appeared in *Nature* 421, 711, 2003)

Droplets of Cartesian Product Operators Involving Three Spins (A)

Tri-linear Cartesian product operators are represented by up to four droplets (τ_1, τ_2, τ_3, τ_4) in the LISA basis. Here, the DROPS representation of characteristic Cartesian operators are displayed for the following cases: (a) three identical components, (b-d) two identical components and (e) all components different.

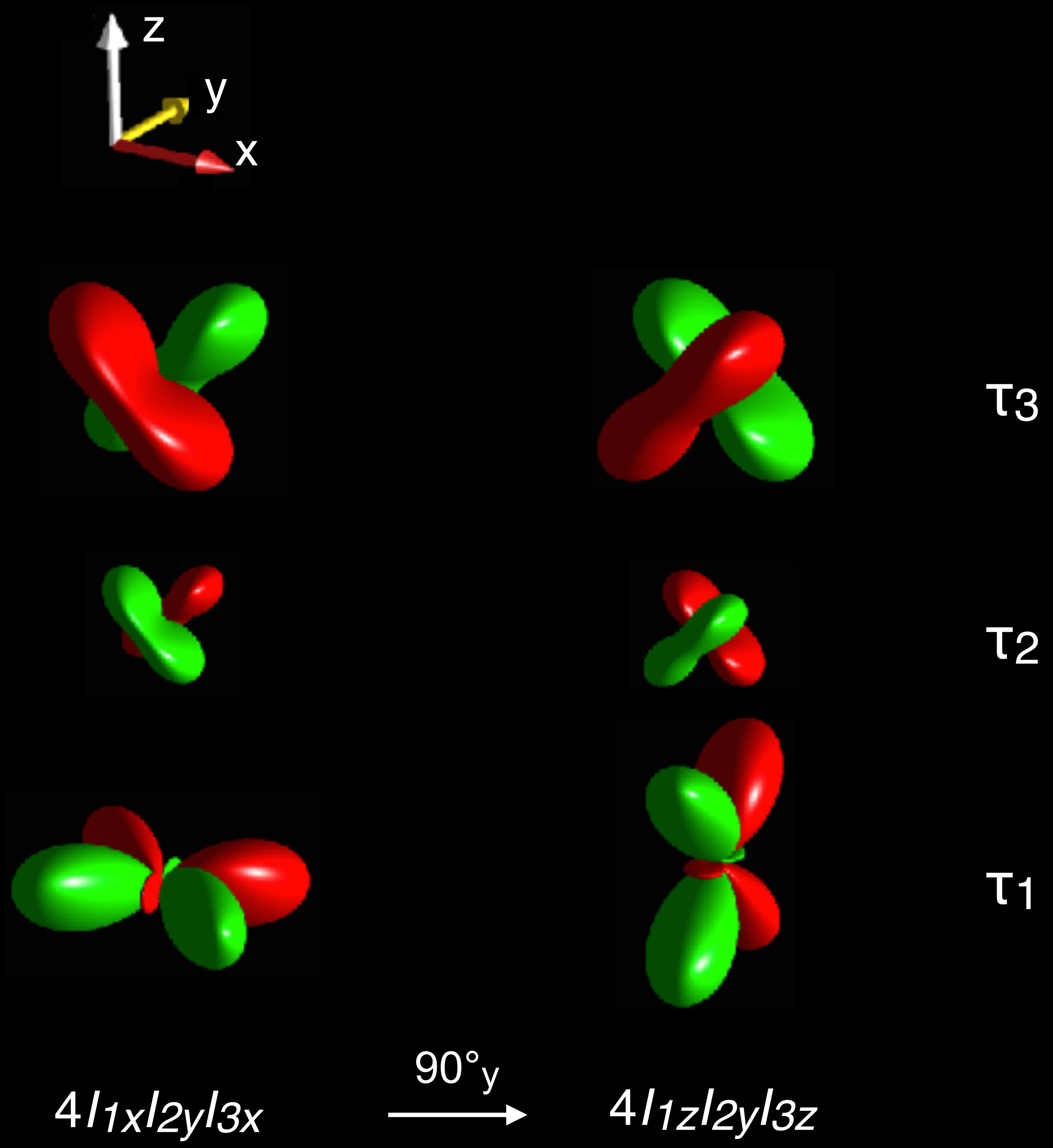


(a) $4I_{1x}I_{2x}I_{3x}$ (b) $4I_{1x}I_{2x}I_{3y}$ (c) $4I_{1x}I_{2y}I_{3x}$ (d) $4I_{1y}I_{2x}I_{3x}$ (e) $4I_{1x}I_{2y}I_{3z}$

Droplets of Cartesian Product Operators Involving Three Spins (B)

Based on the characteristic droplets for trilinear Cartesian Product operators shown on the previous page, the droplets of the remaining trilinear Cartesian product operator can be obtained by rotations around the *x*, *y*, or *z* axis (up to a possible change of sign, which simply corresponds to a change of colors).

For example, the operator $4I_{1z}I_{2y}I_{3z}$ (where the first and last components are identical) can be obtained from the given operator (c) $4I_{1x}I_{2y}I_{3x}$ by a non-selective 90° rotation around the *y* axis. Hence, the DROPS representation of $4I_{1z}I_{2y}I_{3z}$ can be found by rotating each of the droplets of $4I_{1x}I_{2y}I_{3x}$ by 90° around the *y* axis.



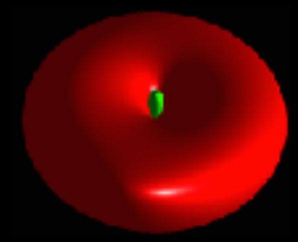
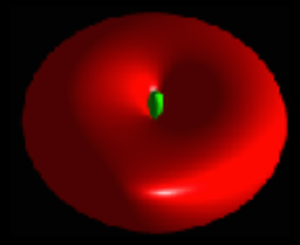
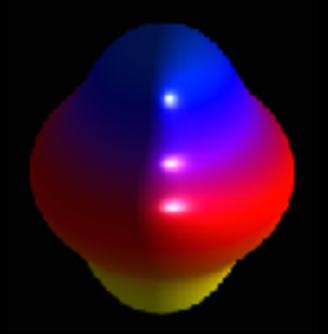
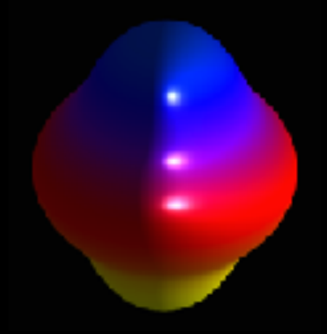
Droplet Symmetry and Coherence Order (A)

The droplet of an operator with *well defined coherence order p* can be easily recognized based on the following rules:

(1) Disregarding the color, the *shape* of the droplet with a well-defined coherence order *p* is invariant under rotations around the *z* axis, i.e. the *shape* is not changed by a *z* rotation.

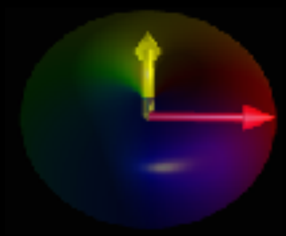
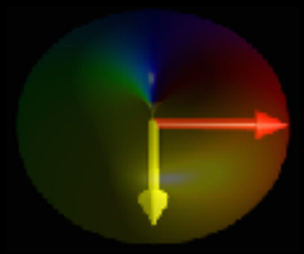
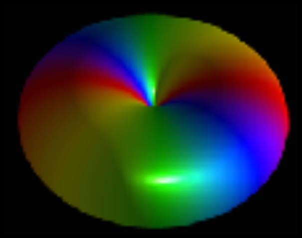
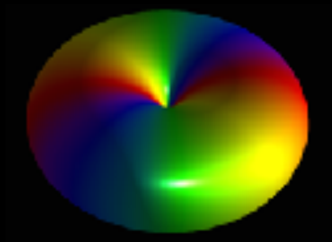
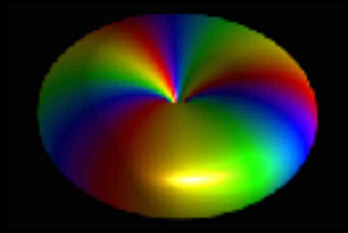
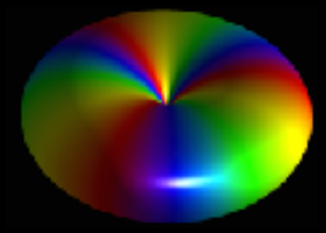
(2) The *coherence order p* of a *droplet can be inferred* from the *color* of a droplet.

(2.1) A droplet of coherence order $p=0$ does not change its color if it is rotated by an arbitrary angle α around the *z* axis, as illustrated by the following two examples.

Operator	*p*	Droplet	*z* Rotation	Droplet
$I_{1x}I_{2x} + I_{1y}I_{2y}$	0		$\xrightarrow{\alpha_z}$	
$I_1^+ I_2^-$	0		$\xrightarrow{\alpha_z}$	

Droplet Symmetry and Coherence Order (B)

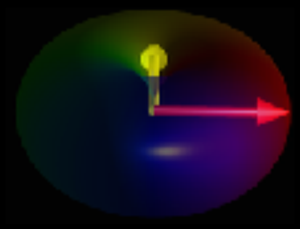
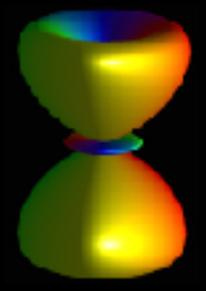
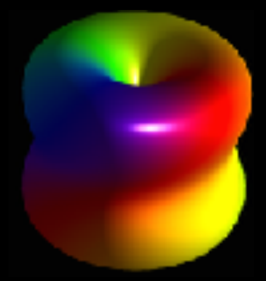
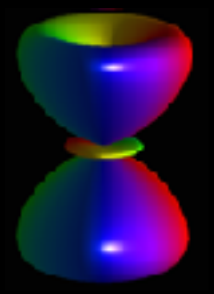
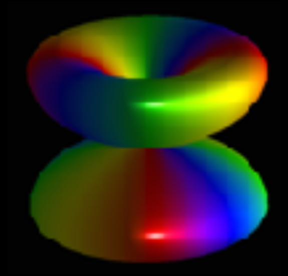
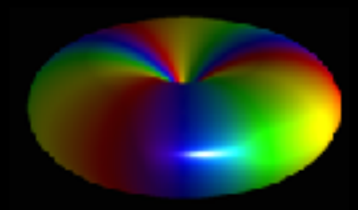
(2.2) A droplet of defined coherence order $p \neq 0$ (where p is a non-zero integer with *either* positive *or* negative sign) is rainbow-colored.
For positive coherence order ($p>0$), the colors change from red to yellow to green to blue when moving counter-clockwise around the droplet.
For negative coherence order, the colors change in the opposite direction, as illustrated by the following examples.

Operator	p	Droplet	Operator	p	Droplet
$I_1^{+} = I_{1x} + \mathrm{i}\, I_{1y}$	+1		$I_1^{-} = I_{1x} - \mathrm{i}\, I_{1y}$	–1	
$I_1^{+} I_2^{+}$	+2		$I_1^{-} I_2^{-}$	–2	
$I_1^{+} I_2^{+} I_3^{+}$	+3		$I_1^{-} I_2^{-} I_3^{-}$	–3	

Droplet Symmetry and Coherence Order (C)

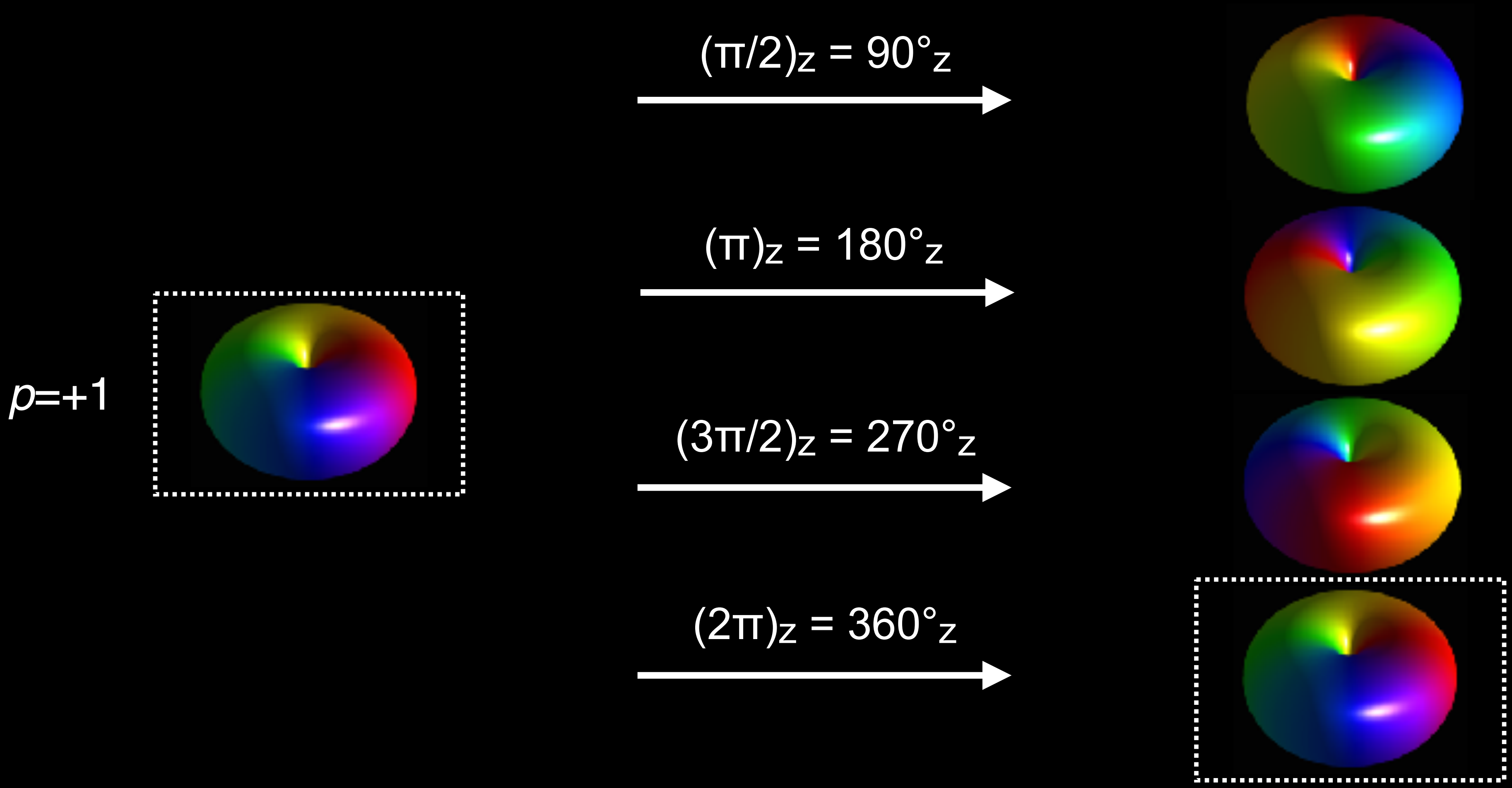
(2.3) For a non-zero, well-defined coherence order *p*, the absolute value $|p|$ of the coherence order of a *droplet* is simply given by the *number of rainbows* encountered when moving once around the *z* axis. (Note that according to (2.2), the *sign* of *p* is given by the *direction*, one has to walk around the *z* axis, in order to move from red to yellow to green to blue.)

Examples:

Droplet	*p*	Droplet	*p*
	+1		–1
	+1		+1
	–2		-3

Droplet Symmetry and Coherence Order (D)

(2.4) A *droplet* of coherence order p does not change its appearance if it is rotated by integer multiples of $2\pi/p$ around the z axis. In the example shown below, $p=+1$ and hence rotations by integer multiples of $2\pi/(+1)= 2\pi =360°$ leave the droplet invariant.



$p=+1$

$(\pi/2)_z = 90°_z$

$(\pi)_z = 180°_z$

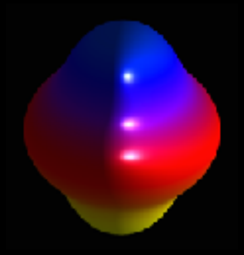
$(3\pi/2)_z = 270°_z$

$(2\pi)_z = 360°_z$

Droplet Symmetry and Coherence Order (E)

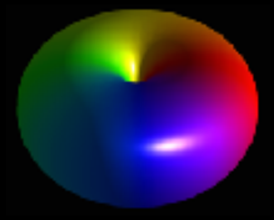
As stated in (2.4), a *droplet* of coherence order $p \neq 0$ does not change its appearance if it is rotated by integer multiples of $2\pi/p$ around the z axis. (Note that for $p=0$, the droplet can be rotated by *any* angle around the z axis without changing its shape or color, as stated in properties (1) and (2.1).) This is illustrated by the examples shown below for well-defined coherence orders p of 0, +1, +2, and +3.

$p=0$



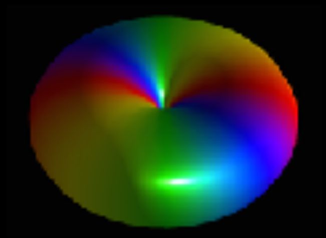
Invariant under *any* z rotation.

$p=+1$



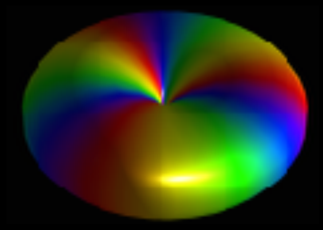
Invariant under $\pm360^\circ_z$, $\pm720^\circ_z$, …

$p=+2$



Invariant under $\pm180^\circ_z$, $\pm360^\circ_z$, …

$p=+3$

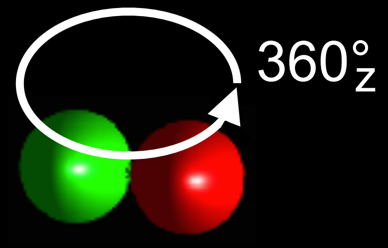


Invariant under $\pm120^\circ_z$, $\pm240^\circ_z$, $\pm360^\circ_z$,…

Droplet Symmetry and Coherence Order (F)

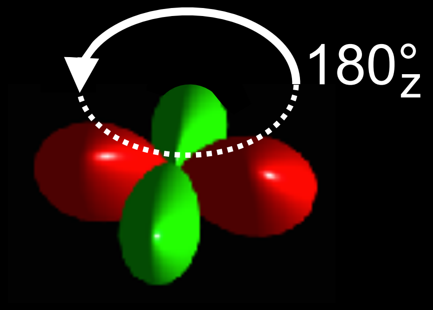
(2.5) Hermitian operators containing a *mixture* of coherence orders ±p (such as ±2) with $|p| \neq 0$, it is still true that the corresponding droplets do not change their appearance if they (or the corresponding operators) are rotated by integer multiples of $2\pi/p = 360°/p$ around the z axis. This is illustrated by the examples shown below for coherence orders p of ±1, ±2, and ±3.

$p = \pm 1$



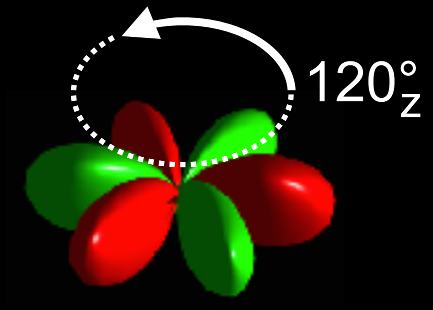
Invariant under $\pm 360°_z$, $\pm 720°_z$, …

$p = \pm 2$



Invariant under $\pm 180°_z$, $\pm 360°_z$, …

$p = \pm 3$

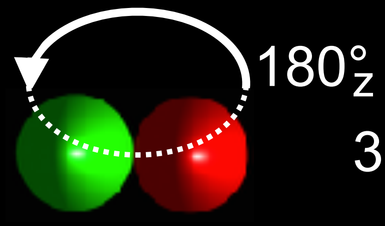


Invariant under $\pm 120°_z$, $\pm 240°_z$, …

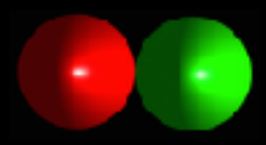
Droplet Symmetry and Coherence Order (G)

(2.6) Hermitian operators corresponding to a *mixture* of coherence orders ±p (such as ±2) with $|p| \neq 0$, change sign if they are rotated by $360°/(2\cdot p)$ around the *z* axis. Hence, after the rotation the shape of the droplet is unchanged but green lobes are now where corresponding red lobes were before the rotation. This is illustrated by the examples shown below for coherence orders *p* of ±1, ±2, and ±3.

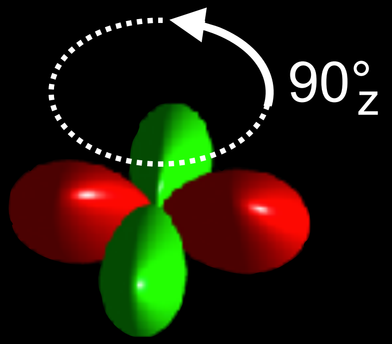
$p=\pm1$



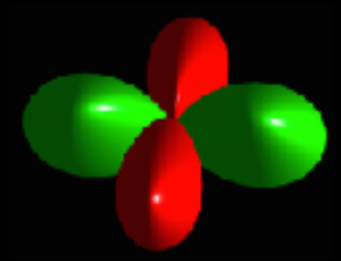
$360°/(2\cdot(\pm1)) = \pm180°$ z rotation:



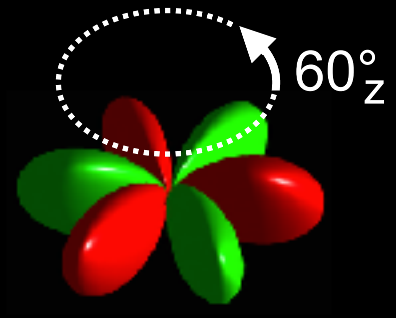
$p=\pm2$



$360°/(2\cdot(\pm2)) = \pm90°$ z rotation:



$p=\pm3$

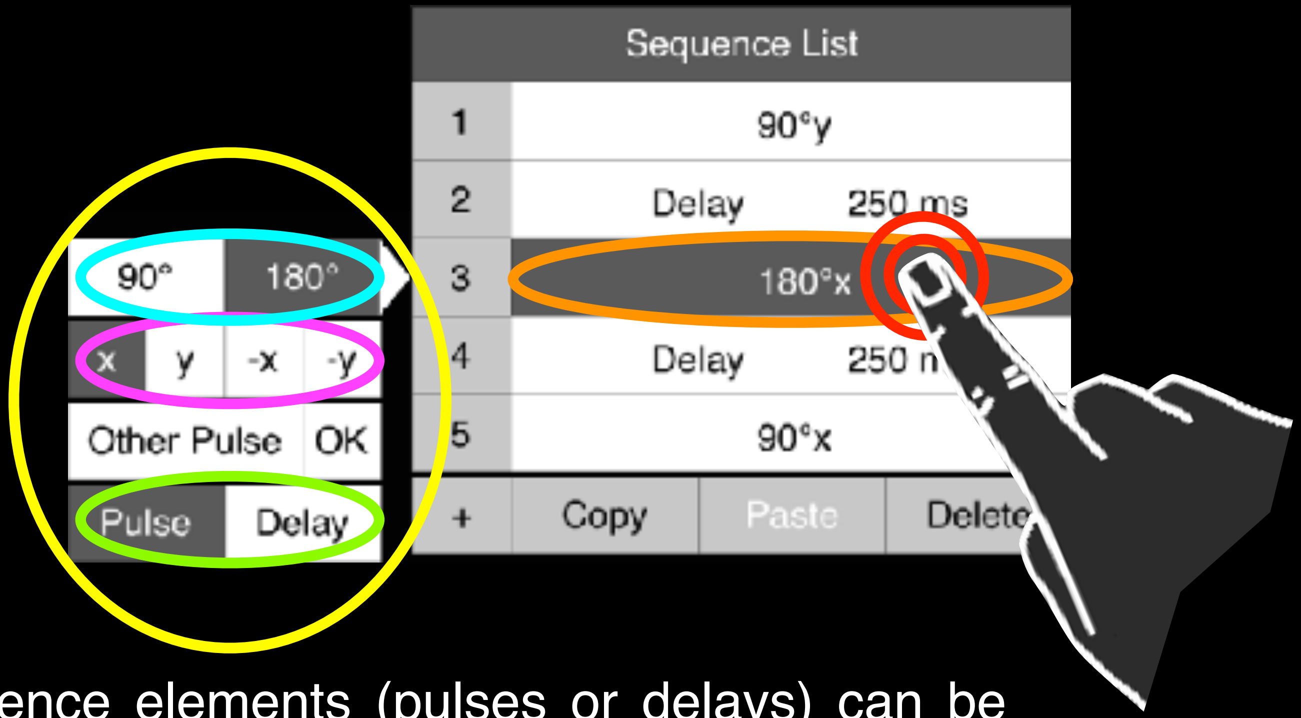


$360°/(2\cdot(\pm3)) = \pm60°$ z rotation:

Pulse Sequence Editor

Pulse Sequence Editor

With a little practice, it is easy to modify existing sequences or to build a new pulse sequence from scratch using the sequence editor. New sequence elements can be created and existing sequence elements can be changed, multiplied (copy/paste) or moved to different positions in the sequence. In order to change or multiply a sequence element, it needs to be activated.

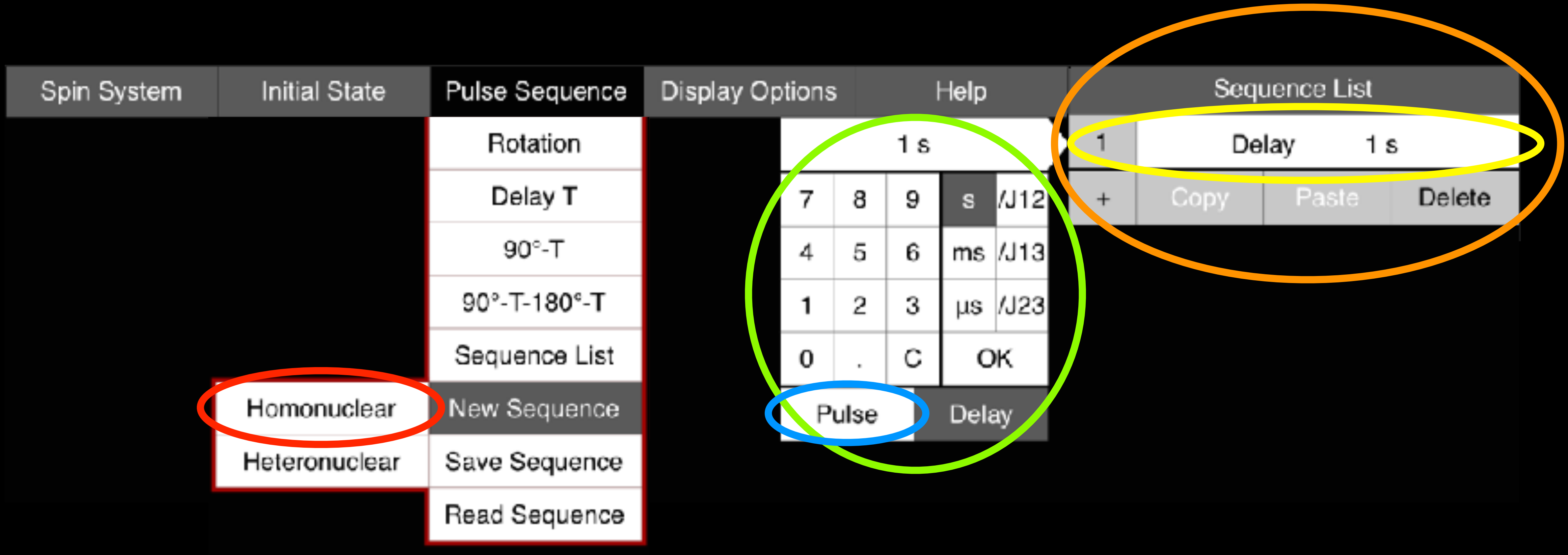


Sequence List	
1	90°y
2	Delay 250 ms
3	180°x
4	Delay 250 n
5	90°x

Activation of a pulse sequence element: Sequence elements (pulses or delays) can be activated by a *double tap*. In the example shown here, sequence element #3 (a 180°_x pulse) has been activated (orange ellipse). You can also activate a sequence element by a double tap in the sequence plot. (If the sequence plot is not visible at the bottom of the screen, select *Display Options > Plot Sequence*.) The activation of a sequence element opens an associated input panel.

Modification of a sequence element: Using the associated input panel of an activated sequence element allows you to change a delay to a pulse or vice versa (green ellipse), modify the flip angle (blue ellipse) and phase (magenta ellipse) of a pulse, or to change the duration of a delay. The duration of delays can be defined in absolute time units (“s”, “ms”, “µs”) or in multiples of the inverse coupling constants, e.g. 0.5/J12=1/(2 J12).

New Homonuclear Sequence (A)

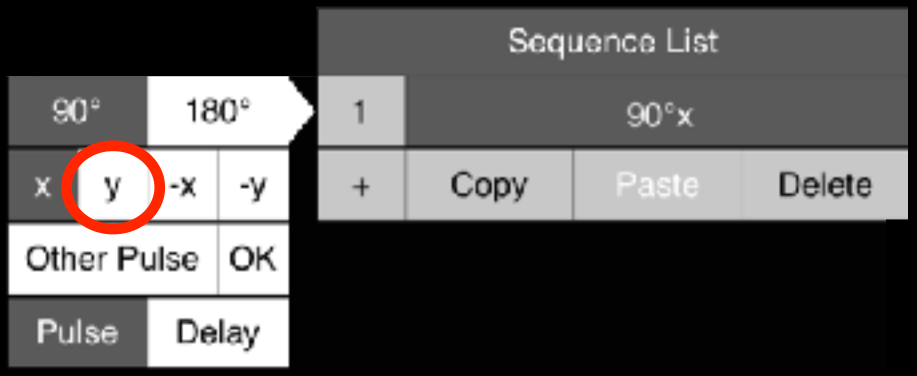


You can build a new pulse sequence using the sequence editor. Let's assume you want to create the homonuclear sequence

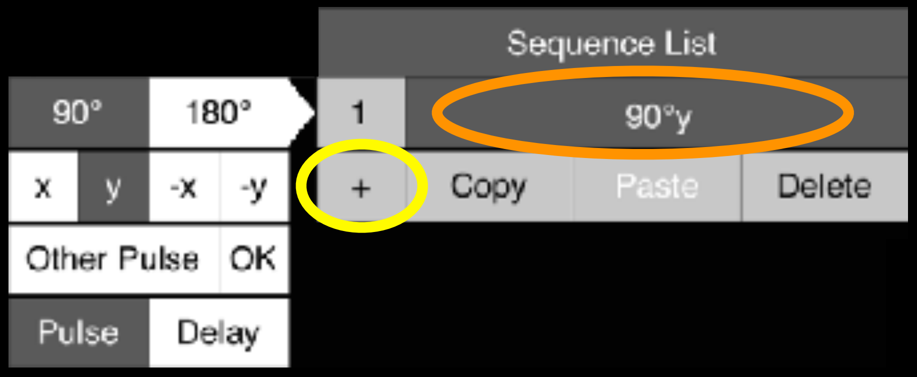
$$90^\circ_y - 250\ \mathrm{ms} - 180^\circ_x - 250\ \mathrm{ms}.$$

Choose *New Sequence* > *Homonuclear* (red ellipse). This will display the *Sequence List* panel (orange ellipse). By default, the new sequence consists of a single entry, a *Delay* of 1 second (yellow ellipse). The current list entry can be modified by the associated input panel (green ellipse), which is displayed at the left of the sequence list. To change the delay to a pulse, touch *Pulse* (blue ellipse).

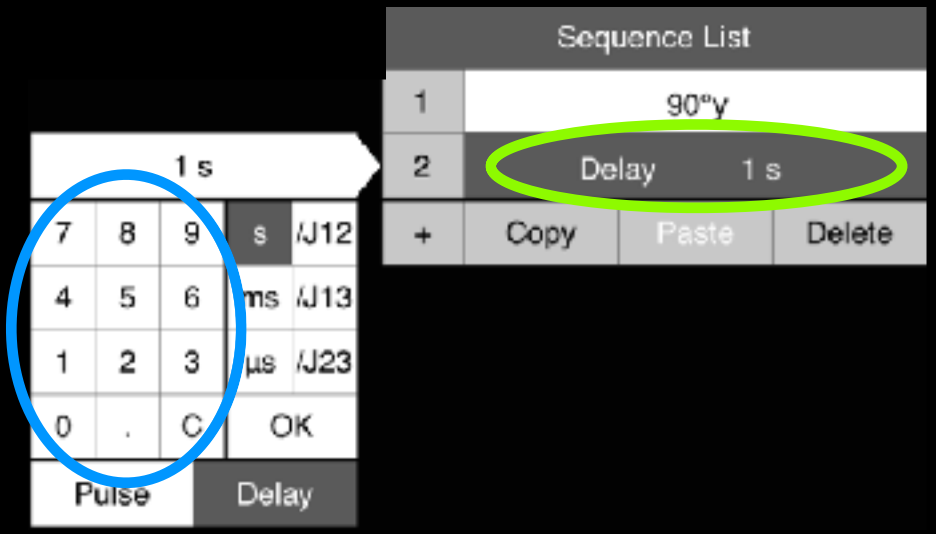
New Homonuclear Sequence (B)



The default pulse is a 90°$_x$. In order to change it to 90°$_y$, touch y (red ellipse).

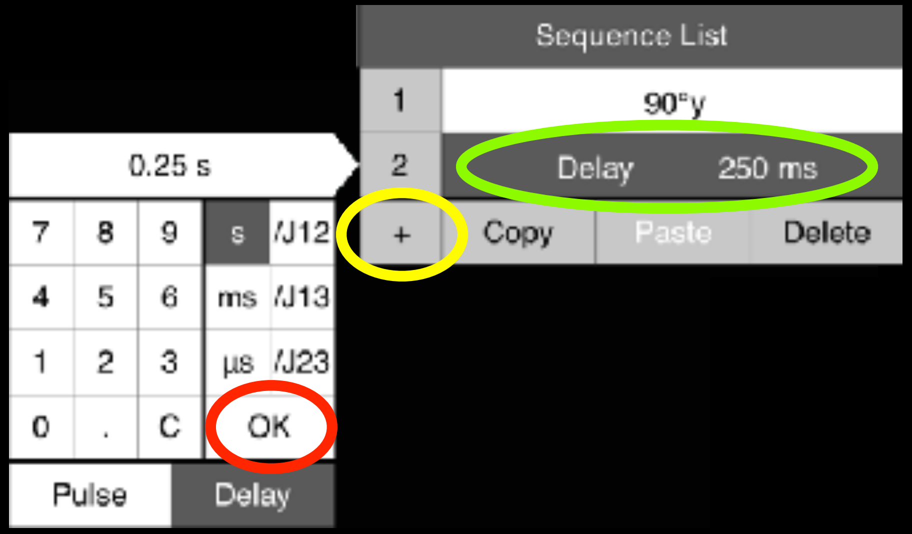


This changes the entry of the sequence list to 90°$_y$ (orange ellipse). In order to add another entry to the *Sequence List*, touch the “+” button (yellow ellipse).



This creates a second entry in the sequence list, which by default is a *Delay* of 1s (green ellipse). The dark background of the second list entry indicates that this is the “active” list entry. (Tip: An inactive list element with a white background can be activated by a *double tap*). To change the delay from 1s to 250 ms = 0.25 s, enter “.25” in the input panel (blue ellipse).

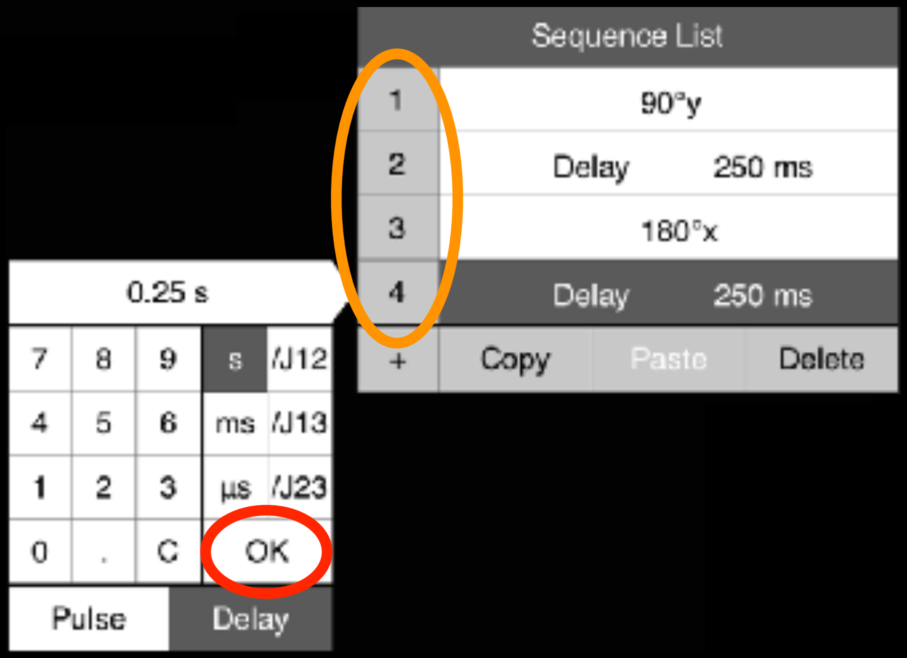
New Homonuclear Sequence (C)



Entering ".25" in the input panel changes the second list entry to 250 ms. (Alternatively, you could enter "250" and touch "ms" to achieve the same result.)

Add a third list entry by touching the "+" button (yellow ellipse) and change it to a180°_x pulse.

Finally, add another delay of 250 ms by creating a new list entry using the "+" button and changing the entry to 250 ms as before.

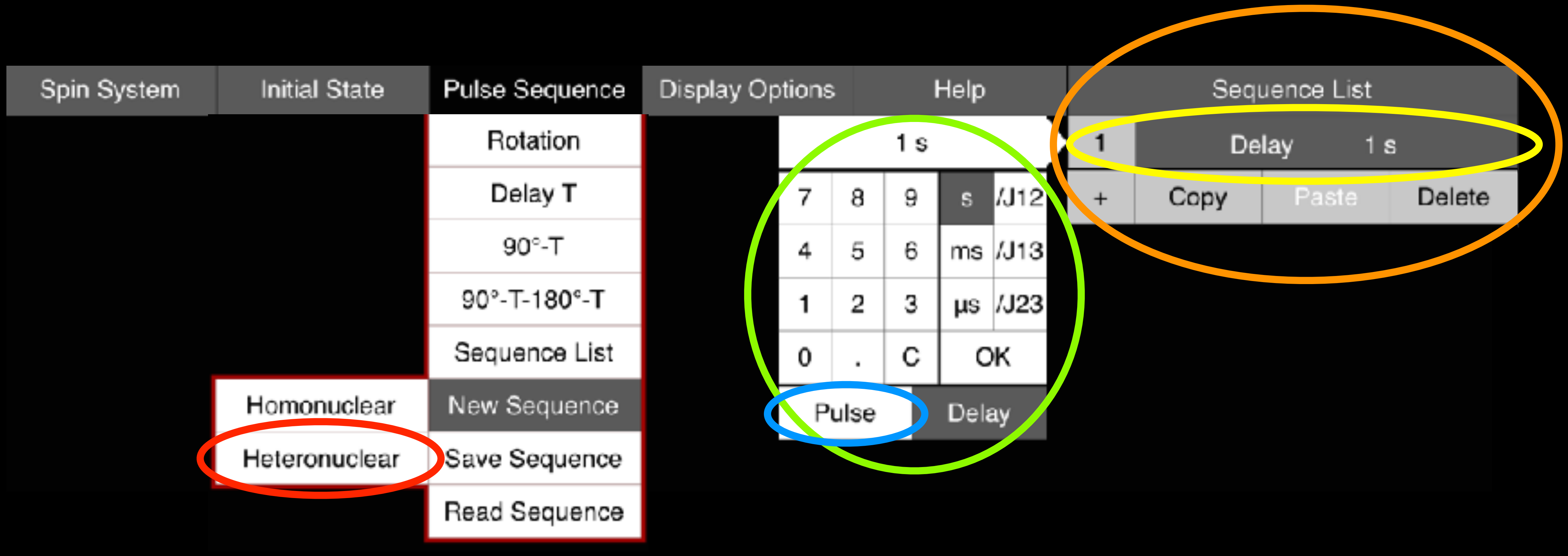


This completes the creation of the sequence 90°_y - 250 ms - 180°_x - 250 ms.

Tip: To close the input panel, touch the *OK* button (red ellipse).

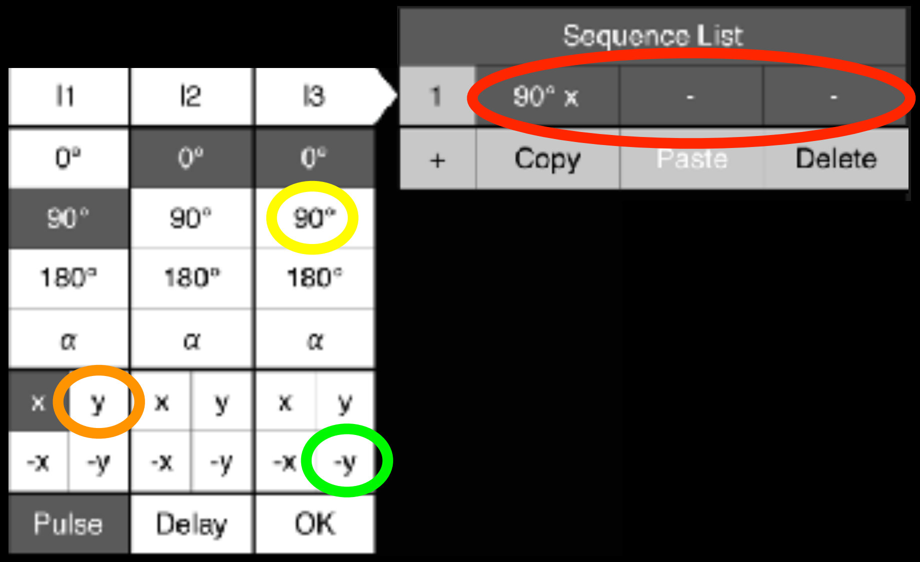
Tip: Explore also alternative ways to create the same pulse sequence. Additional editing tools include *Copy*, *Paste* and the option to move pulse sequence elements to a new position by dragging the position number of the sequence element (orange ellipse).

New Heteronuclear Sequence (A)



To create a new heteronuclear sequence with spin-selective pulses, select *New Sequence > Heteronuclear* (red ellipse). As in the homonuclear case, this will display the *Sequence List* panel (orange ellipse) and by default the new sequence consists of a *Delay* of 1 s (yellow ellipse). To change the delay to one (or several) selective pulses, touch *Pulse* (blue ellipse) on the input panel (green ellipse).

New Heteronuclear Sequence (B)



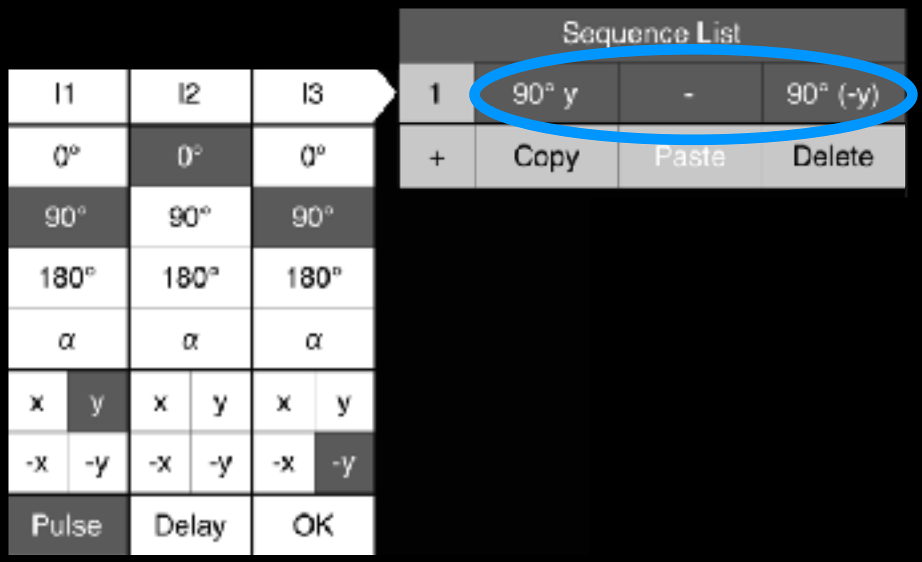
Sequence List

1	90° x	-	-

In the heteronuclear case, the default pulse is $90°_x(I_1)$, i.e. a spin I_1-selective $90°_x$ pulse (red ellipse).

Suppose the first pulse sequence element should be an I_1-selective $90°_y$ pulse which is applied simultaneously with an I_3-selective $90°_{-y}$ pulse.

To create this pulse sequence element, first select phase “y” for the I_1-selective 90° pulse (orange ellipse). Then select 90° for the flip angle of the I_3-selective pulse (yellow ellipse) and finally select phase “–y” for this pulse (green ellipse).



Sequence List

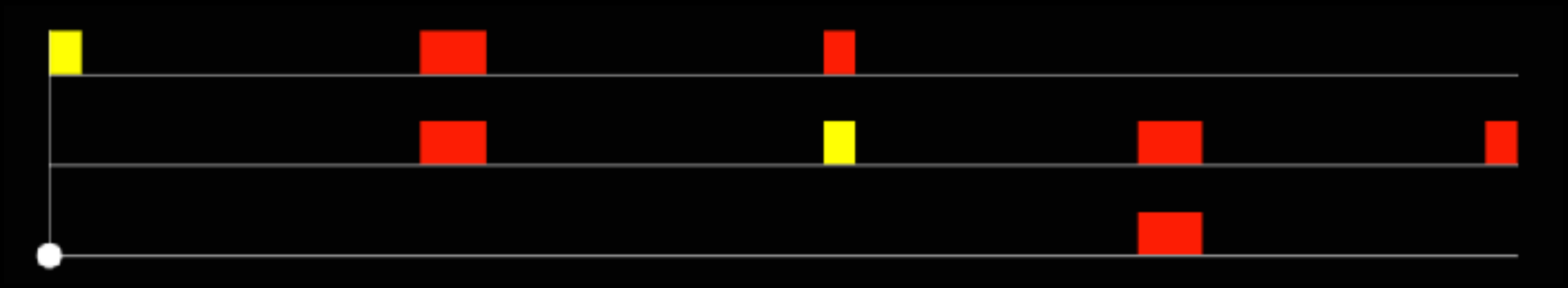
1	90° y	-	90° (-y)

As shown in the *Sequence List*, (blue ellipse), the first sequence element consists of a simultaneous $90°_y(I_1)$ and a $90°_{-y}(I_3)$ pulse.

Tip: Rather than building pulse sequences from scratch, you can also edit existing sequences by choosing *Display Options > List/Edit Seq.* or by “activating” a desired element of the graphically displayed pulse sequence by a *double tap*.

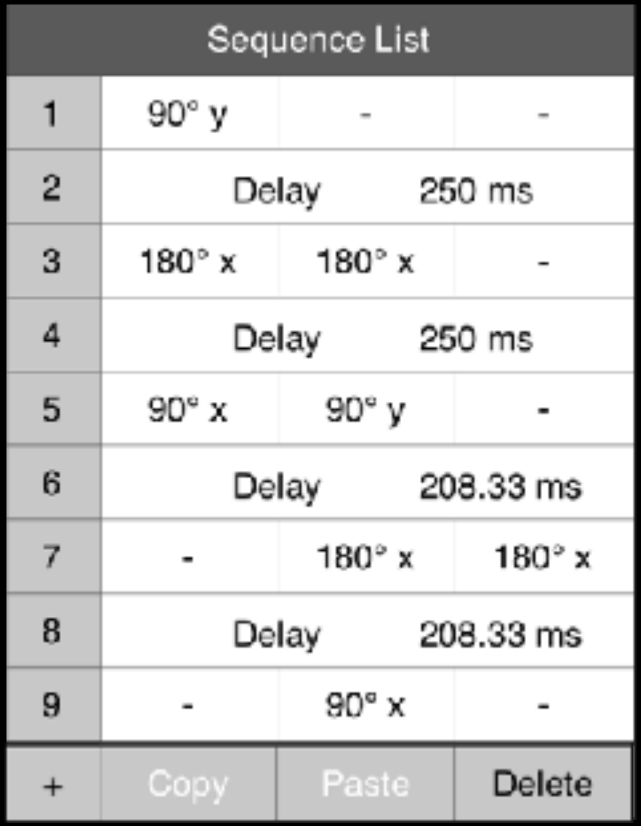
Modifying an Existing Pulse Sequence (A)

Let us consider the sequence *Pulse Sequence > Sequence List > Heterouclear > z1–> zzz* shown graphically below. Pulses that act selectively on spins I_1, I_2 or I_3 are displayed in the first, second or third row, respectively.



It is also possible to display a list of the individual pulse sequence elements by choosing *Display Options > List/Edit Seq*. (see list shown at the right).

This heteronuclear pulse sequence consists of seven pulse sequence elements, which are consecutively numbered in the left column of the list. Elements 1, 3, 5, 7, and 9 are spin-selective pulses, where the first, second, and third column corresponds to I_1-, I_2-, and I_3-selective pulses. Elements 2, 4, 6, and 8 are delays.

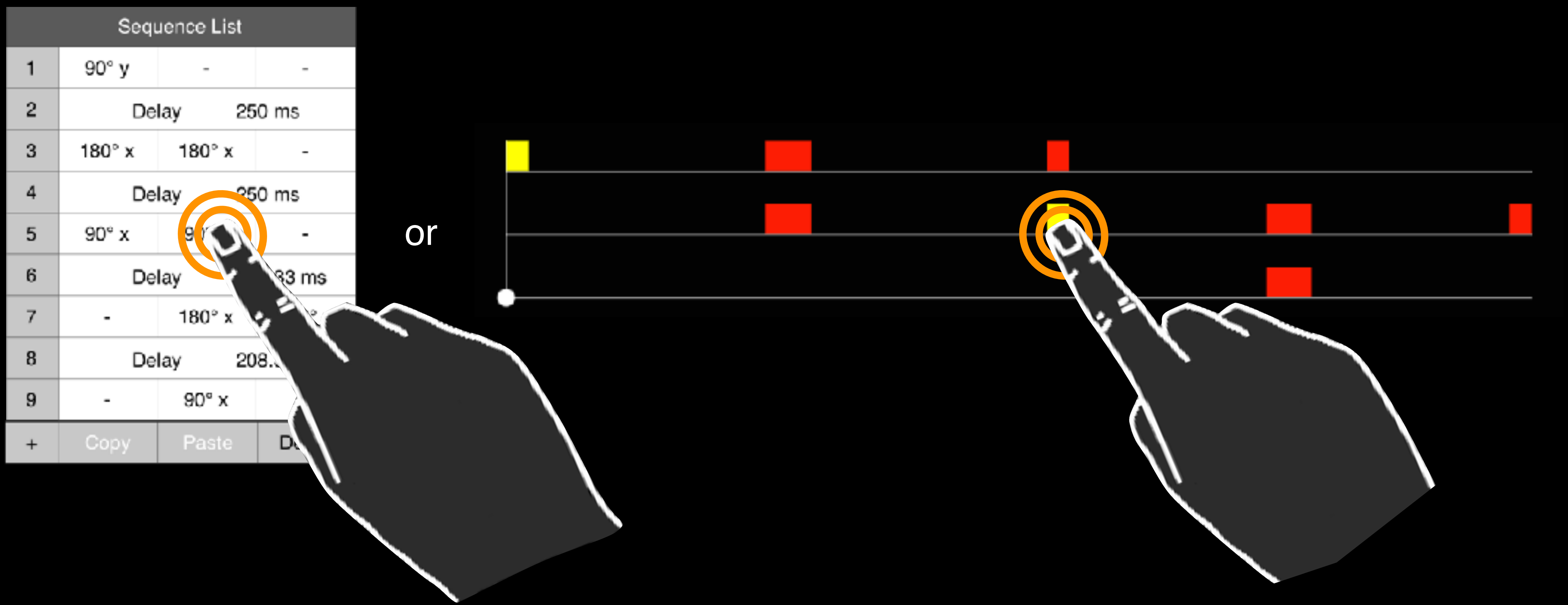


Sequence List

1	90° y	-	-
2	Delay	250 ms	
3	180° x	180° x	-
4	Delay	250 ms	
5	90° x	90° y	-
6	Delay	208.33 ms	
7	-	180° x	180° x
8	Delay	208.33 ms	
9	-	90° x	-

Modifying an Existing Pulse Sequence (B)

In order to modify a given pulse sequence element, it must be "activated", which can be achieved either by *double tapping* with a single finger the pulse sequence element in the *Sequence List* or by *double tapping* it in the sequence plot:



Sequence List

1	90° y	-	-
2		Delay	250 ms
3	180° x	180° x	-
4		Delay	250 ms
5	90° x	9	-
6		Delay	33 ms
7	-	180° x	
8		Delay	208.
9	-	90° x	
+	Copy	Paste	D

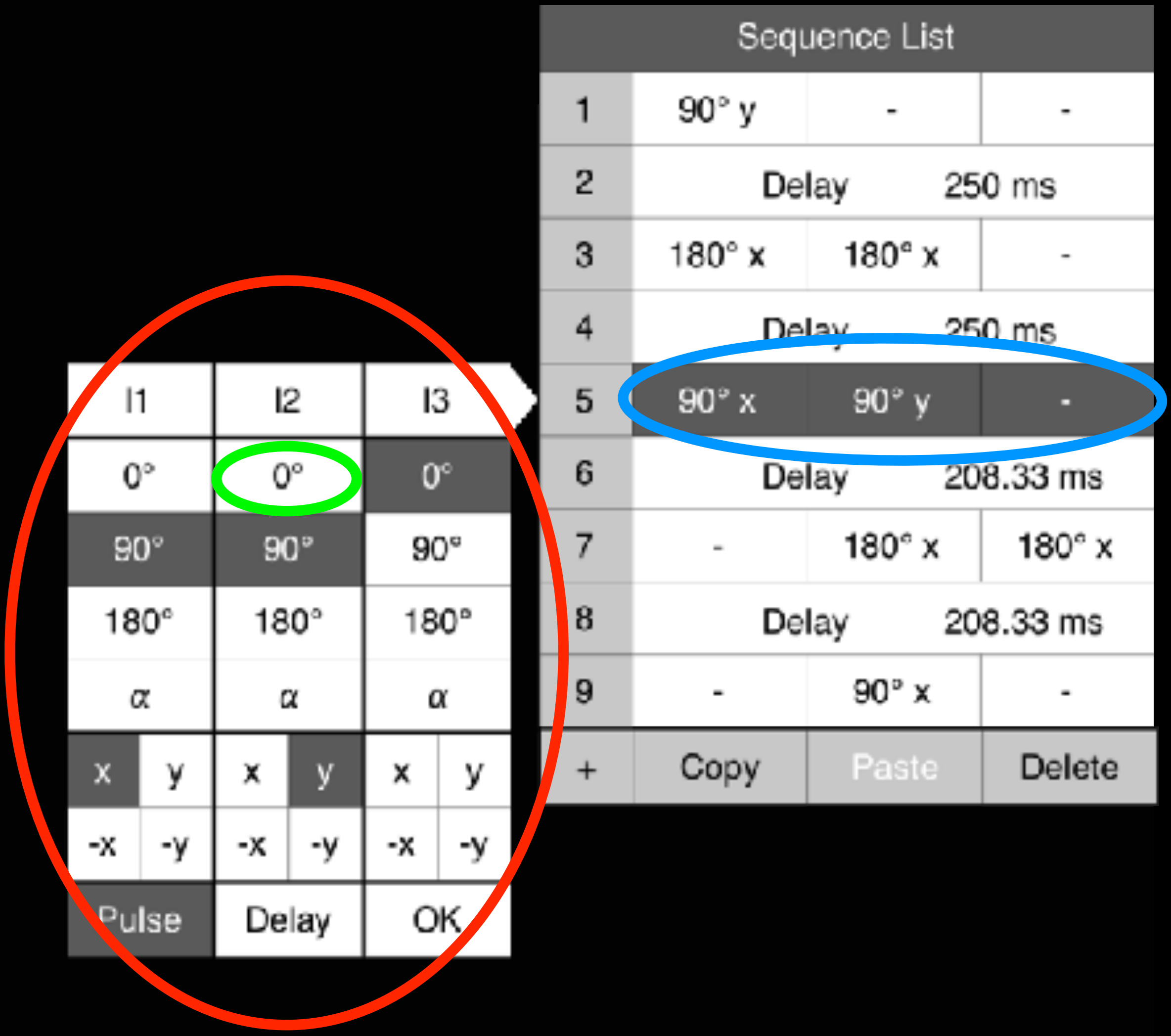
As shown on the next page, the activated pulse sequence element (in this example, element 5) is highlighted in the *Sequence List* by white letters on a dark background and in the sequence plot by bold white lines (see next page).

Modifying an Existing Pulse Sequence (C)

In the example, the highlighted "active" pulse sequence element is indicated by dark and light blue ellipses in the sequence list and in the sequence plot, respectively.

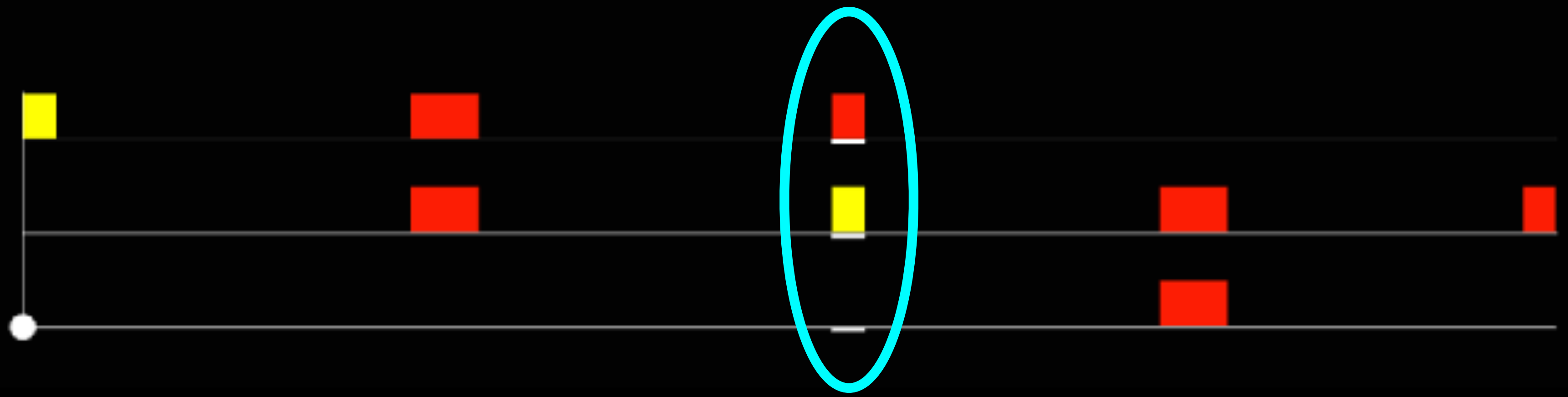
The associated input panel (red ellipse) allows you to modify the active pulse sequence element.

For example, the I2-selective 90°y pulse can be eliminated by choosing a flip angle of 0° (green ellipse).



Sequence List

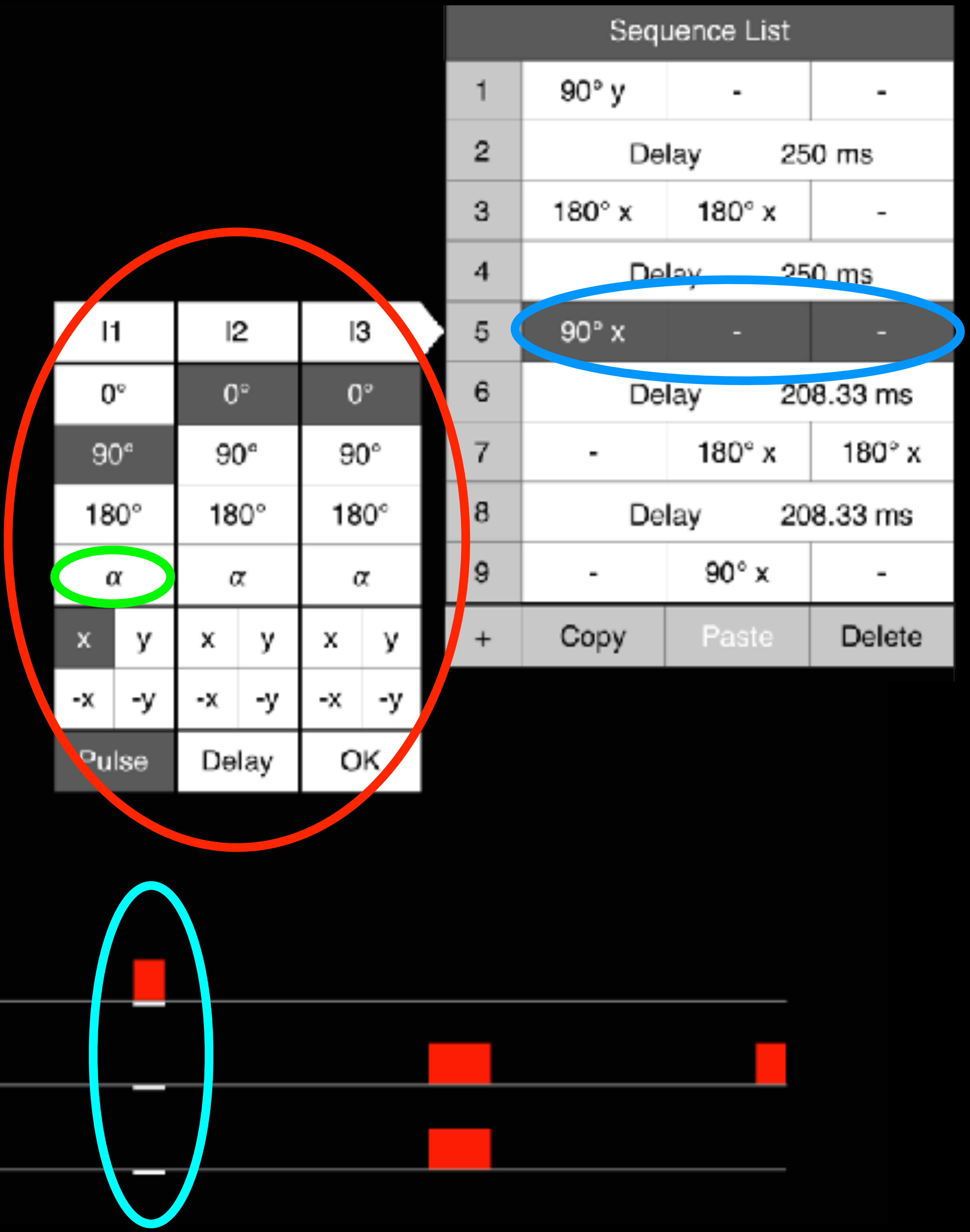
1	90° y	-	-
2	Delay	250 ms	
3	180° x	180° x	-
4	Delay	250 ms	
5	90° x	90° y	-
6	Delay	208.33 ms	
7	-	180° x	180° x
8	Delay	208.33 ms	
9	-	90° x	-



Modifying an Existing Pulse Sequence (D)

The modification is instantly displayed both in the sequence list and in the sequence plot (dark and light blue ellipses, respectively).

It is also possible to choose a flip angle different from the most common values (90° or 180°) by touching "α" (green ellipse). As shown on the next page, this will open an additional input panel that allows you to numerically enter a desired flip angle.



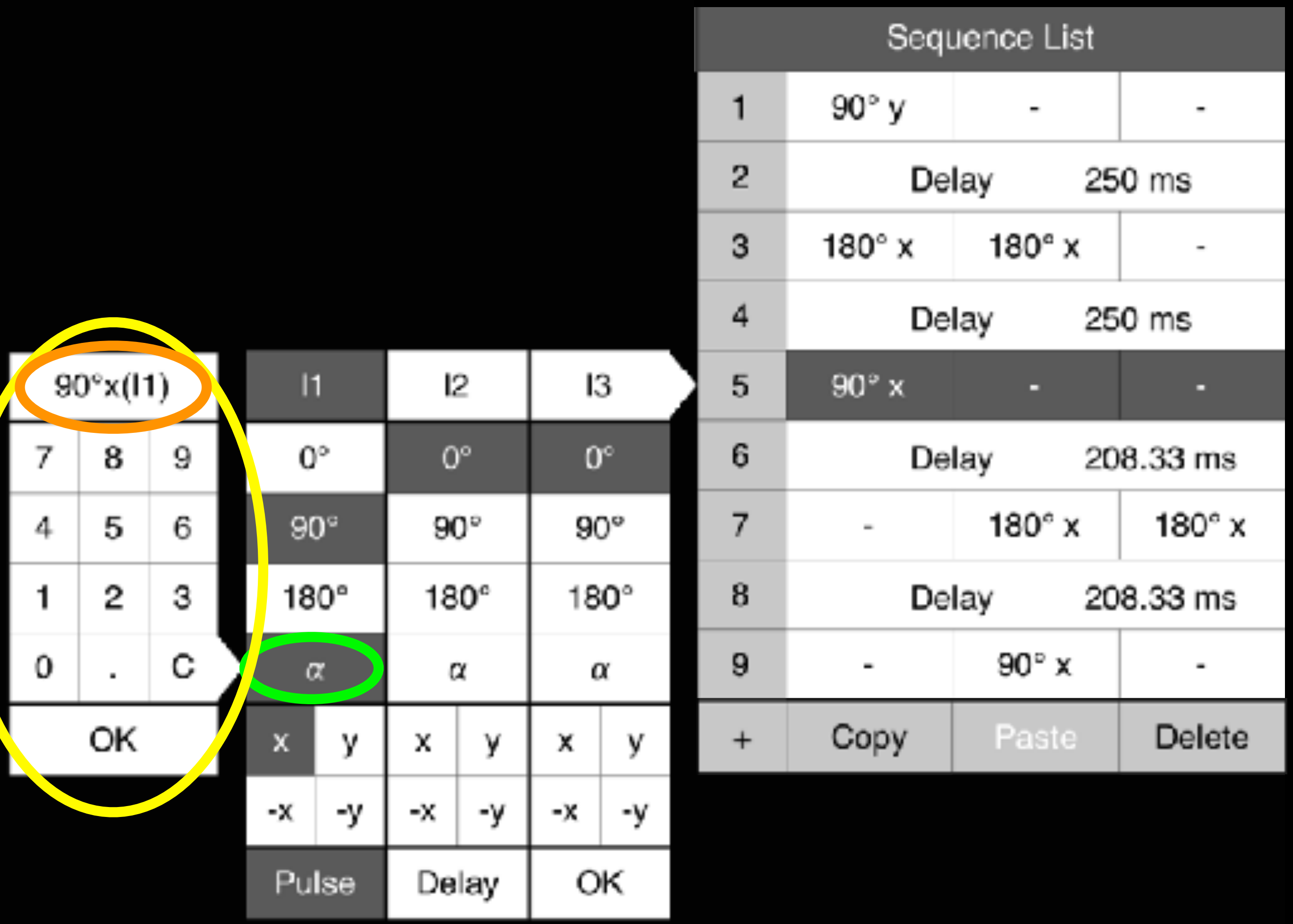
Sequence List

1	90° y	-	-
2	Delay	250 ms	
3	180° x	180° x	-
4	Delay	250 ms	
5	90° x	-	-
6	Delay	208.33 ms	
7	-	180° x	180° x
8	Delay	208.33 ms	
9	-	90° x	-
+	Copy	Paste	Delete

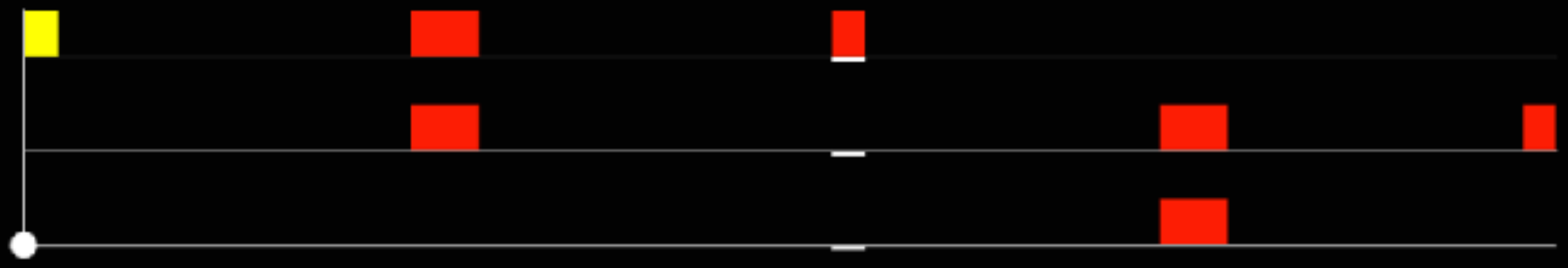
Modifying an Existing Pulse Sequence (E)

Touching the “α” button (green ellipse) opens the additional input panel (yellow ellipse). The display “90°x(I1)” at the top (orange ellipse) shows the current flip angle (90°) of the spin I_1-selective pulse with phase x.

For example, we can change the flip angle to 60° by touching the corresponding keys of the input panel. The result is shown on the next page.



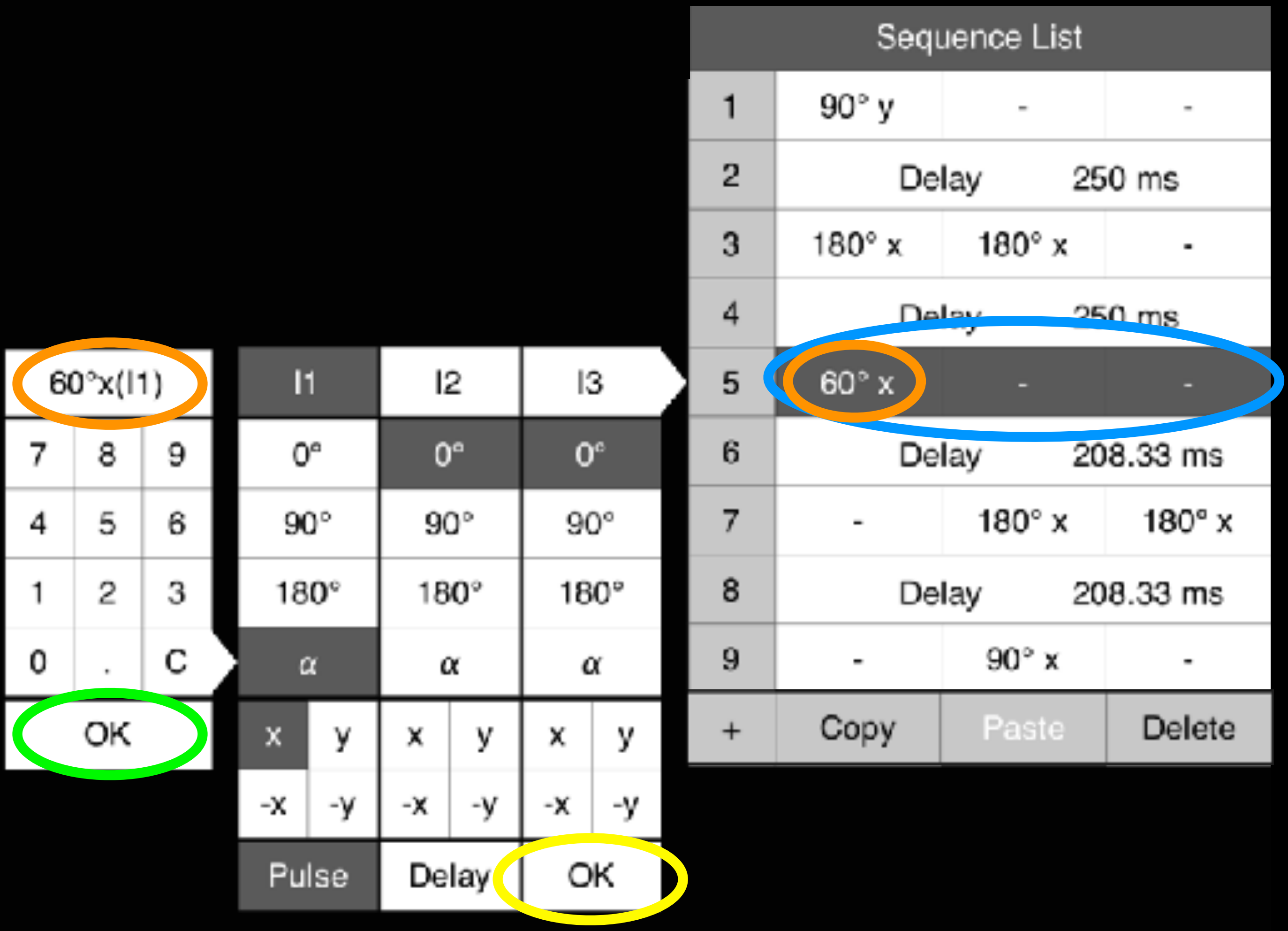
Sequence List			
1	90° y	-	-
2	Delay	250 ms	
3	180° x	180° x	-
4	Delay	250 ms	
5	90° x	-	-
6	Delay	208.33 ms	
7	-	180° x	180° x
8	Delay	208.33 ms	
9	-	90° x	-
+	Copy	Paste	Delete



Modifying an Existing Pulse Sequence (F)

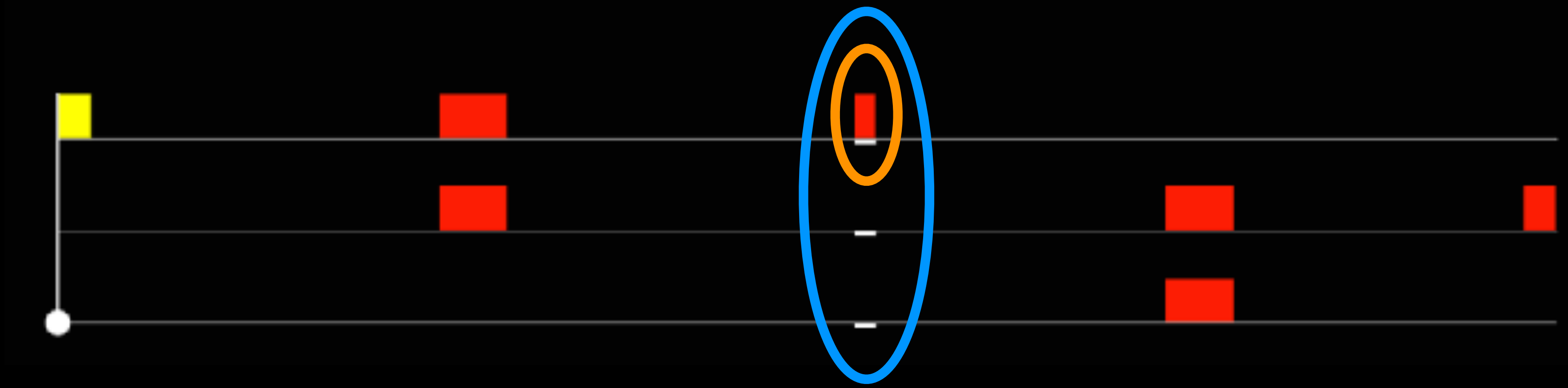
The new flip angle of 60° is displayed numerically in the Sequence List as well as graphically in the sequence plot (orange ellipses).

The additional input panel at the left can be closed with the *OK* button (green ellipse). The input panel in the center can be closed and the currently “active” pulse sequence element (blue ellipses) can be “deactivated” by touching the *OK* button of the center panel (yellow ellipse), see next page.

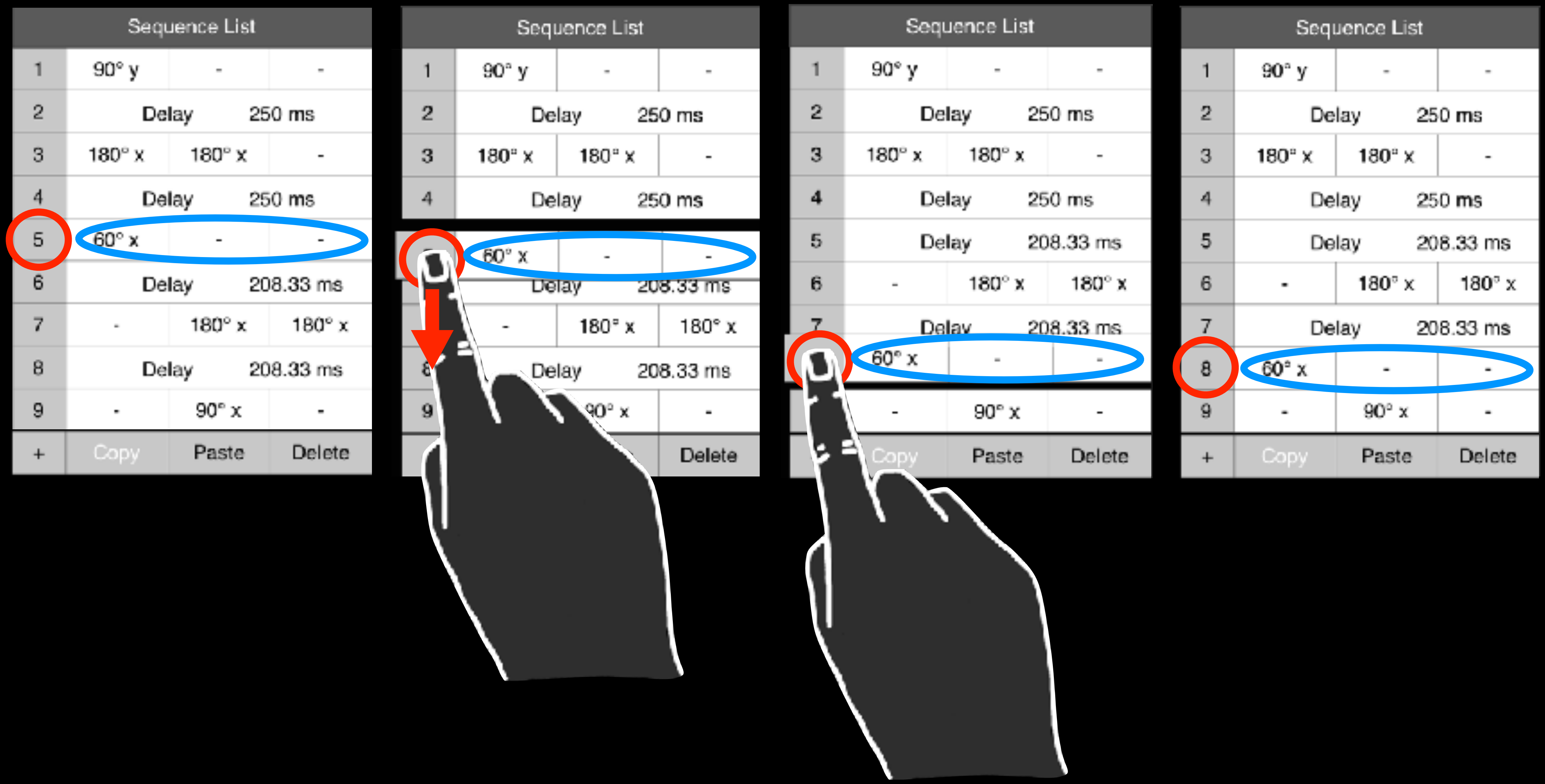


Sequence List

1	90° y	-	-
2		Delay	250 ms
3	180° x	180° x	-
4		Delay	250 ms
5	60° x	-	-
6		Delay	208.33 ms
7	-	180° x	180° x
8		Delay	208.33 ms
9	-	90° x	-
+	Copy	Paste	Delete



Moving Sequence Elements to Different Positions



Sequence List			
1	90° y	-	-
2	Delay	250 ms	
3	180° x	180° x	-
4	Delay	250 ms	
5	60° x	-	-
6	Delay	208.33 ms	
7	-	180° x	180° x
8	Delay	208.33 ms	
9	-	90° x	-
+	Copy	Paste	Delete

Sequence List			
1	90° y	-	-
2	Delay	250 ms	
3	180° x	180° x	-
4	Delay	250 ms	
	60° x	-	-
	Delay	208.33 ms	
	-	180° x	180° x
8	Delay	208.33 ms	
9		90° x	-
			Delete

Sequence List			
1	90° y	-	-
2	Delay	250 ms	
3	180° x	180° x	-
4	Delay	250 ms	
5	Delay	208.33 ms	
6	-	180° x	180° x
7	Delay	208.33 ms	
	60° x	-	-
	-	90° x	-
	Copy	Paste	Delete

Sequence List			
1	90° y	-	-
2	Delay	250 ms	
3	180° x	180° x	-
4	Delay	250 ms	
5	Delay	208.33 ms	
6	-	180° x	180° x
7	Delay	208.33 ms	
8	60° x	-	-
9	-	90° x	-
+	Copy	Paste	Delete

A sequence element (blue ellipse) is moved by touching its entry number (red circle) and dragging it to the desired new position. In the example shown above, the I_1-selective 60°_x pulse is moved from position #5 to position #8 of the sequence.

Copy/Paste

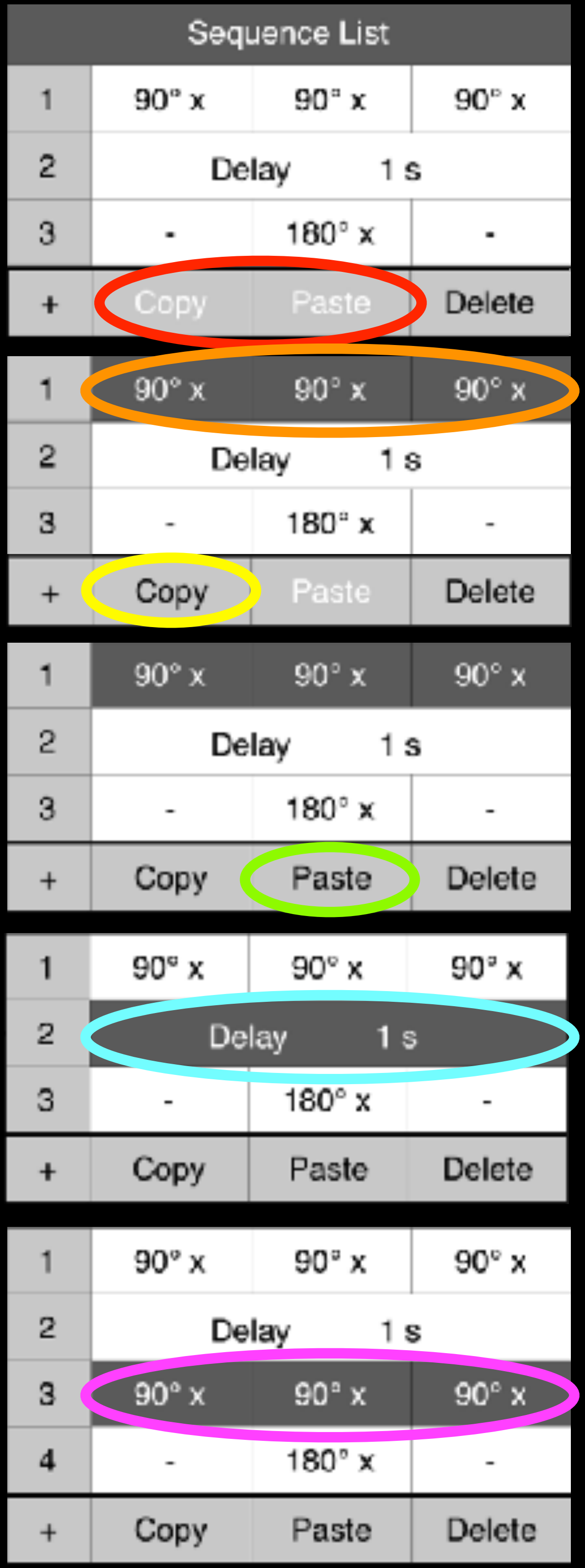
An activated pulse sequence element can be copied and pasted using the corresponding buttons at the bottom of the sequence list. Initially, the *Copy* and the *Paste* buttons are inactive (indicated by a white font, see red ellipse).

Double tapping a sequence element activates not only the selected sequence element (indicated by a white font on dark background, see orange ellipse) but also makes the *Copy* button active (indicated by changing the white font to black, see yellow ellipse).

Touch the *Copy* button to store the active pulse sequence element in an internal buffer. If the buffer is loaded, the *Paste* button become active (indicated by a black font, see green ellipse).

Touching the *Paste* button inserts the stored sequence element *after* the currently activated sequence element. (If no sequence element is activated, the stored sequence element is inserted at the end of the sequence.)

In the example shown on the right, the goal was to copy element #1 and to insert it after element #2. This is achieved by activating element #1 and copying it to the buffer. Then element #2 is activated (blue ellipse) and the stored sequence element is pasted after element #2 at position #3 (magenta ellipse).



Sequence List

1	90° x	90° x	90° x
2	Delay 1 s		
3	-	180° x	-
+	Copy	Paste	Delete

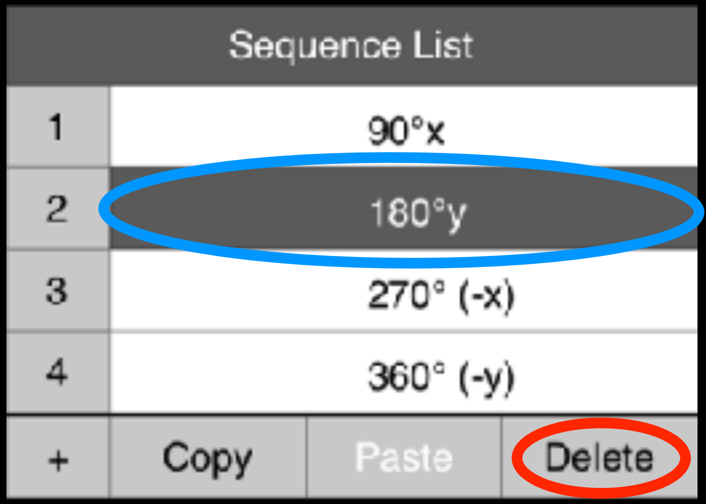
1	90° x	90° x	90° x
2	Delay 1 s		
3	-	180° x	-
+	Copy	Paste	Delete

1	90° x	90° x	90° x
2	Delay 1 s		
3	-	180° x	-
+	Copy	Paste	Delete

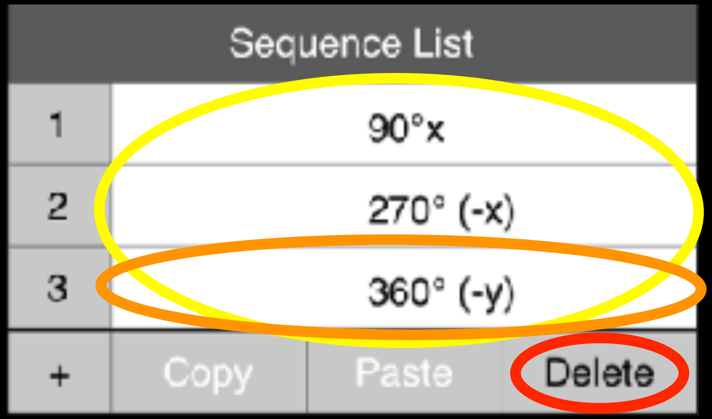
1	90° x	90° x	90° x
2	Delay 1 s		
3	-	180° x	-
+	Copy	Paste	Delete

1	90° x	90° x	90° x
2	Delay 1 s		
3	90° x	90° x	90° x
4	-	180° x	-
+	Copy	Paste	Delete

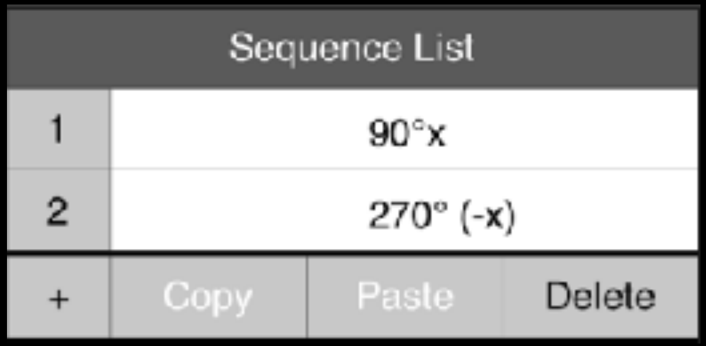
Deleting Sequence Elements



	Sequence List
1	90°x
2	180°y
3	270° (-x)
4	360° (-y)



	Sequence List
1	90°x
2	270° (-x)
3	360° (-y)



	Sequence List
1	90°x
2	270° (-x)

Pulse sequence elements can be deleted by touching the *Delete* button (red ellipse).

If a sequence element is activated (blue ellipse), the *Delete* button removes the activated sequence element from the list. (Remember that a sequence element can be activated by a *double tap*.)

If no element is activated in the sequence list (yellow ellipse), the last sequence element (orange ellipse) of the list is deleted.

Display and Duration of Pulses

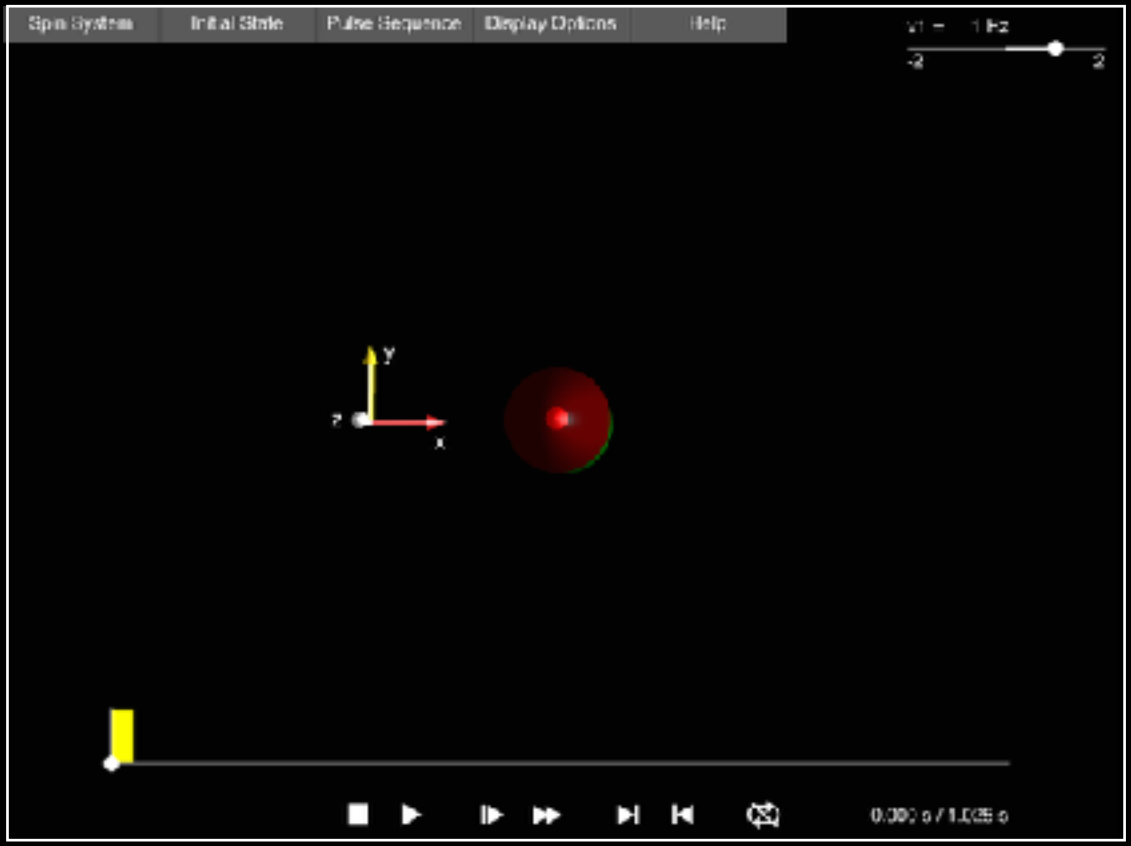
As discussed in the introduction, the simulations in the current version of the *SpinDrops* app are assuming ideal pulses, i.e. the effects of frequency offsets and couplings are not taken into account during the pulses.

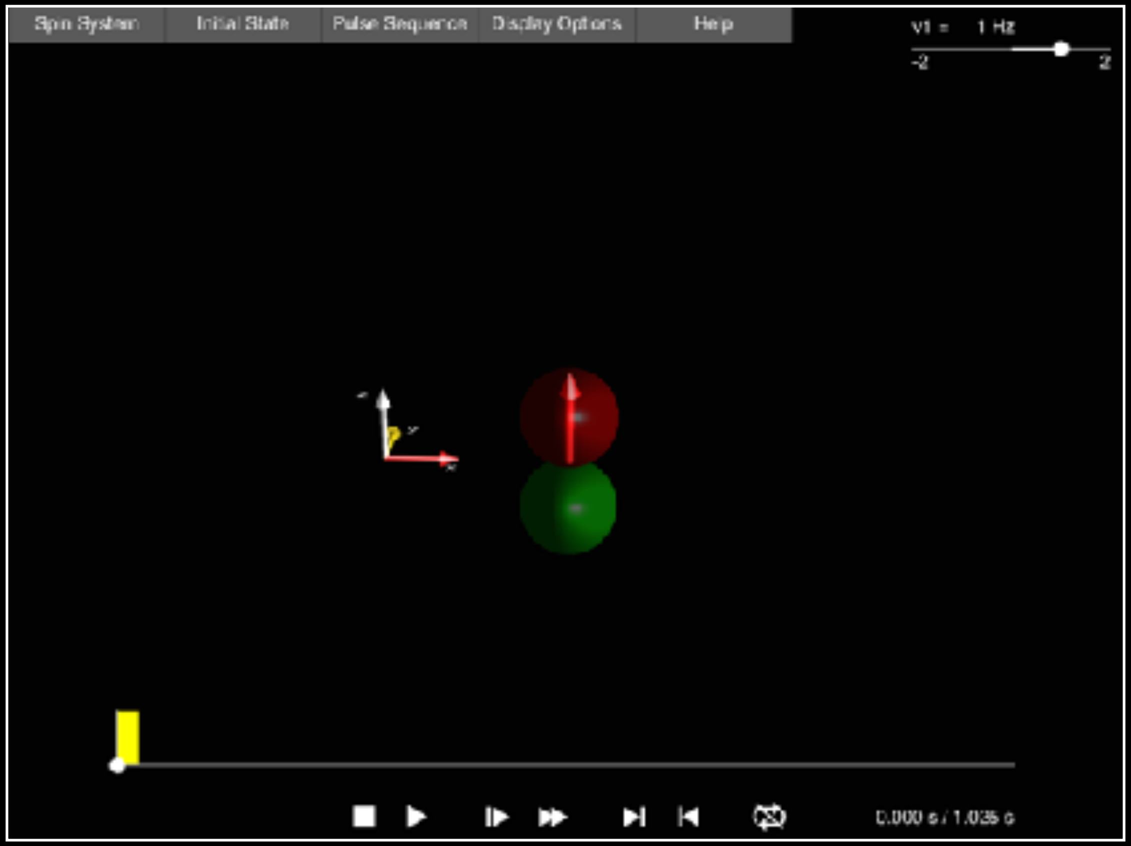
In order to make the pulses visible in the sequence plots and to be able to distinguish pulses of different flip angles based on the width of the displayed rectangles, a low default pulse amplitude (Rabi frequency) of only 10 Hz is assumed. Thus, the duration of a 360° pulse is 1/(10 Hz) = 0.1 s = 100 ms, the duration of a 180° pulse is 50 ms, and the duration of a 90° pulse is 25 ms. However, as frequency offsets and couplings are neglected during the duration of the pulses in the simulations, the pulses have the same effect as ideal delta pulses of negligible duration.

Additional care has to be taken in the case of heteronuclear experiments, where pulses can be selectively applied to individual spins. In this case, it is important to remember that during the duration of a pulse, offsets and couplings do not evolve, even if a particular spin is not irradiated. This is indicated by a dark grey rectangle. Also note that simultaneously applied pulses with different flip angles are displayed with different widths and are centered in the sequence plot. The example at the right shows a zoom of the simultaneous 180°_x (red rectangle) and 45°_y (yellow rectangles) pulses in the DEPT-45 sequence. Note the dark grey rectangle indicating the pulse duration, which has been enhanced here for better visibility.

Examples

Example 1: Excitation and Precession of a Single Spin (A)

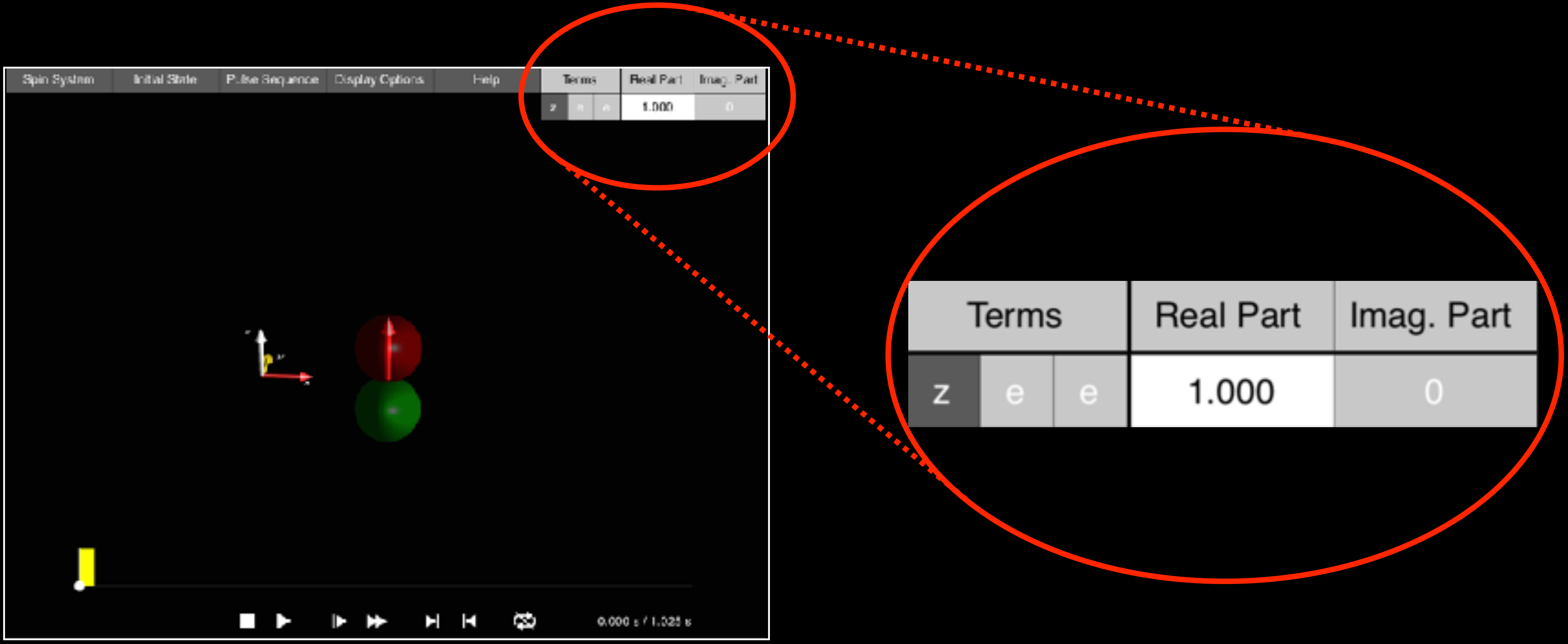




Let us start with a simple example of an uncoupled spin, for which the DROPS display is equivalent to the well-known vector representation. Selecting *Spin System > 1 Spin* should result in the display shown on the top. By default, the initial state is I_{1z} (representing “z magnetization”). The red vector in the transparent red sphere should point along the z axis.

By default, initially, the single spin is seen approximately from the positive z axis. If you prefer, you can choose a different perspective. For example, touching the center of the screen and moving the finger upward, results in the following display. (Using one finger, you can rotate the display like a trackball. For more finger gestures, see *Help > Tutorial*.)

Example 1: Excitation and Precession of a Single Spin (B)



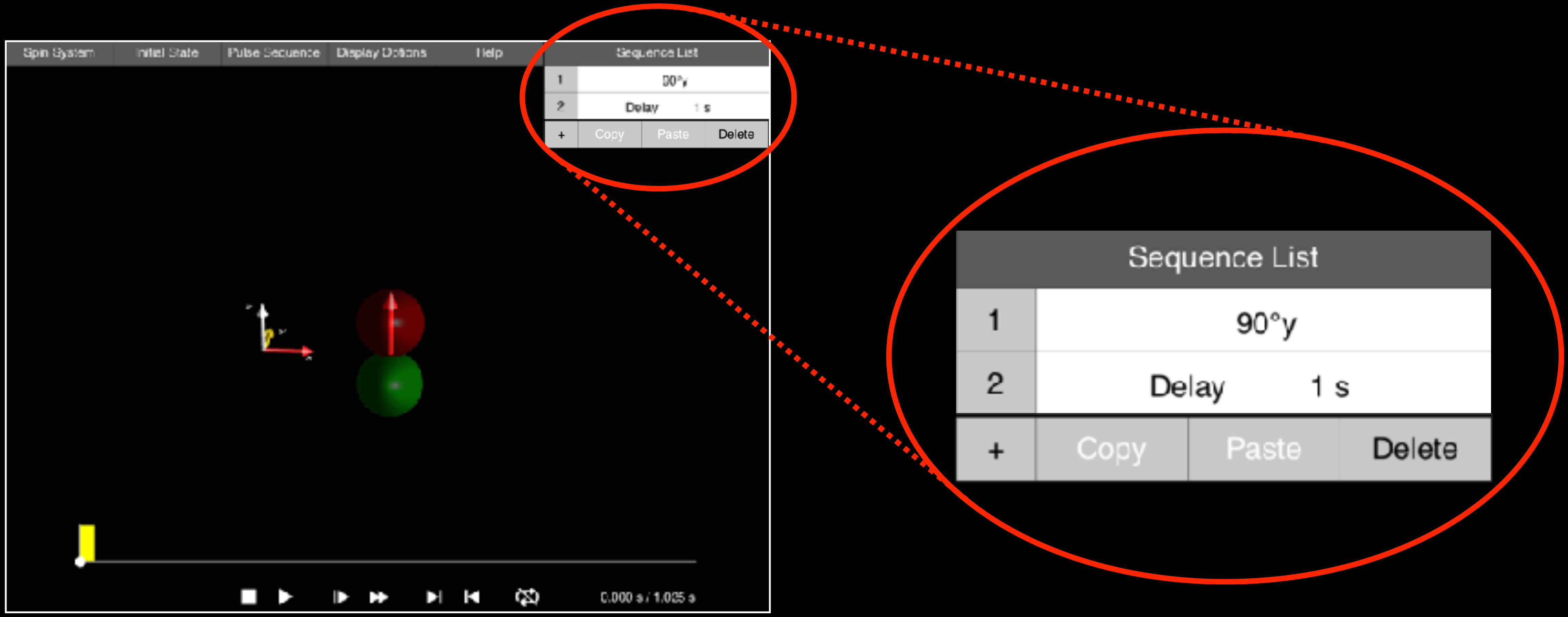
Terms			Real Part	Imag. Part
z	e	e	1.000	0

In order to see the currently displayed product operator, select *Display Options > List Prod. Ops*.

As shown at the top, the list of product operators representing the current state contains only the term zee, corresponding to I_{1z}. Its coefficient has no imaginary part and the real part is 1.

(If a different initial state is shown, select *Initial State > I1z.)*

Example 1: Excitation and Precession of a Single Spin (C)



Sequence List	
1	90°_y
2	Delay 1 s

Also by default, the pulse sequence should be a 90°_y pulse followed by a delay of 1 second. The pulse sequence is displayed schematically at the bottom of the screen, where the 90°_y pulse is represented by a yellow rectangle.

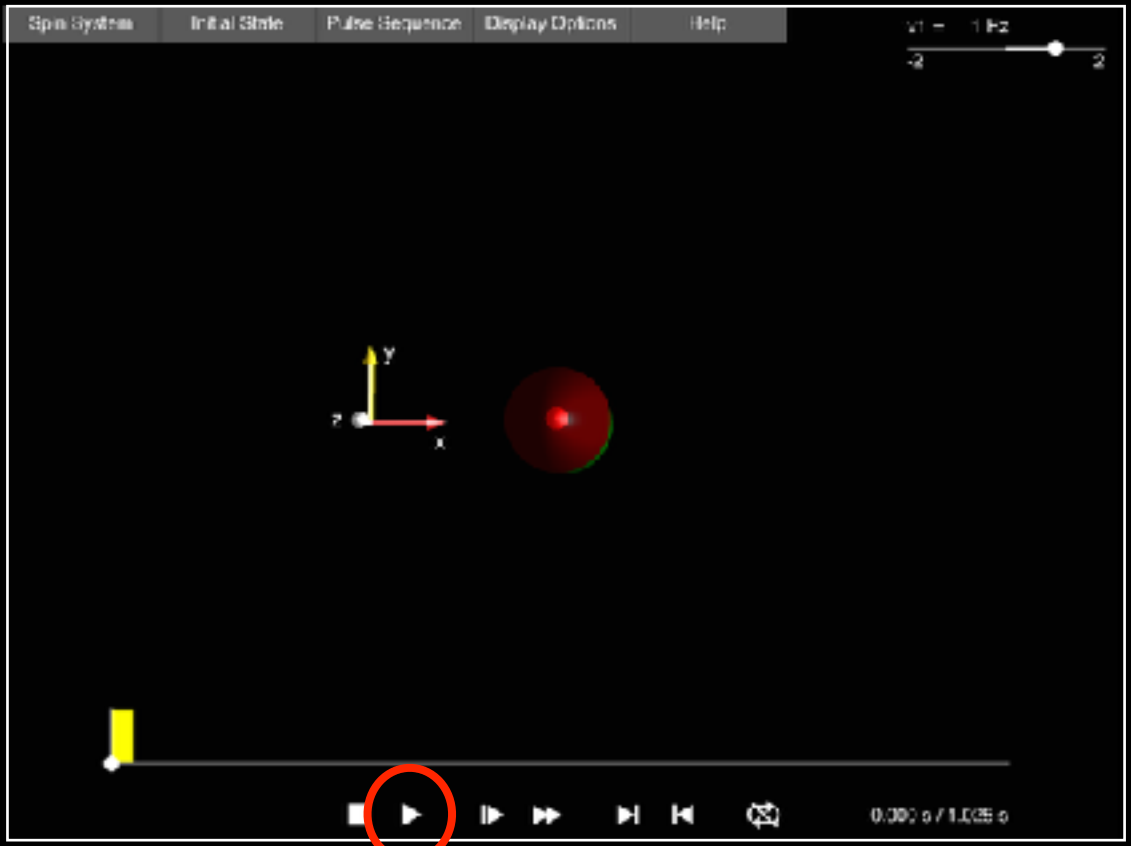
In order to see the detailed parameters of the currently selected pulse sequence, select *Display Options > List/Edit Seq*.
This displays the list shown above. As expected, it consists of two elements: A 90°_y pulse followed by a delay of 1 second. If a different pulse sequence is listed, select *Pulse Sequence > 90°-T > T=1s*.

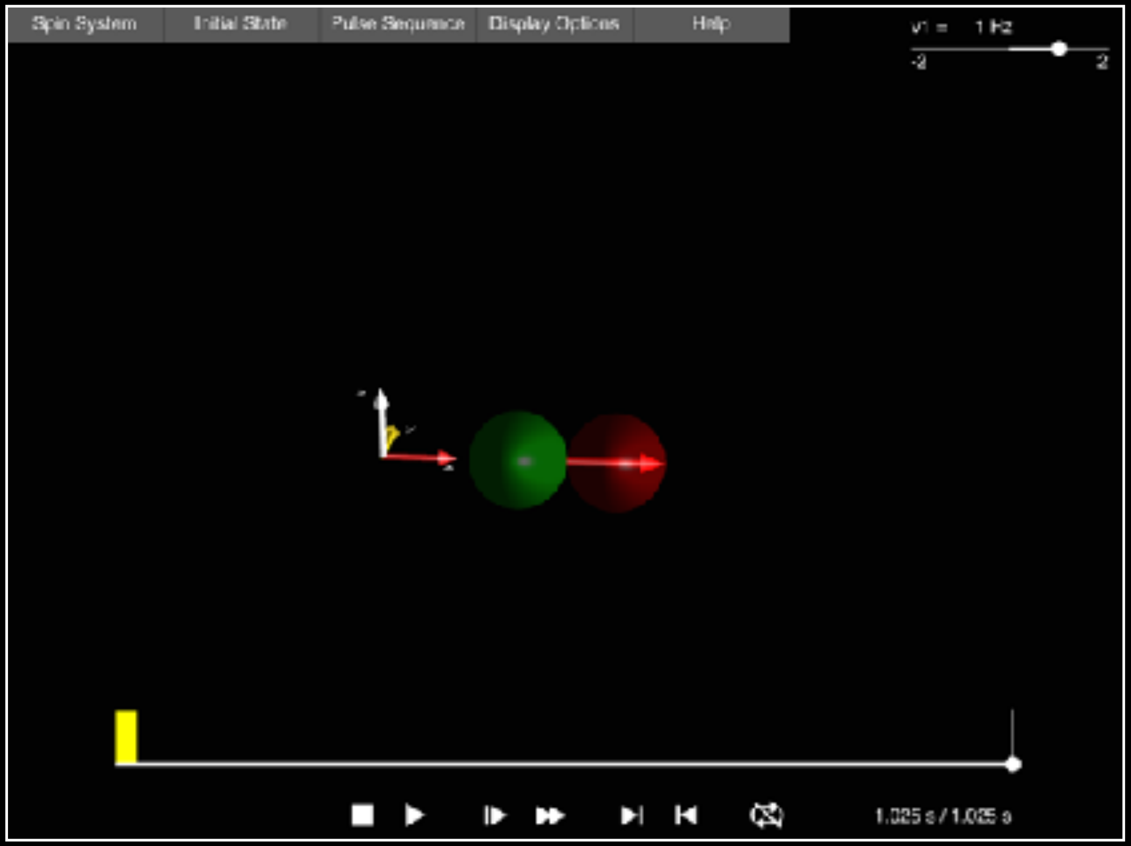
Example 1: Excitation and Precession of a Single Spin (D)

By default, the offset frequency of the spin I_1 is ν_1 = 1 Hz. This can be checked (or modified) by selecting *Spin System > Parameters*.

The displayed parameter and its current value is indicated above the slider: “v1 = 1 Hz”. The allowed range of the values (here from –2 to 2) is indicated below the slider.

Example 1: Excitation and Precession of a Single Spin (E)

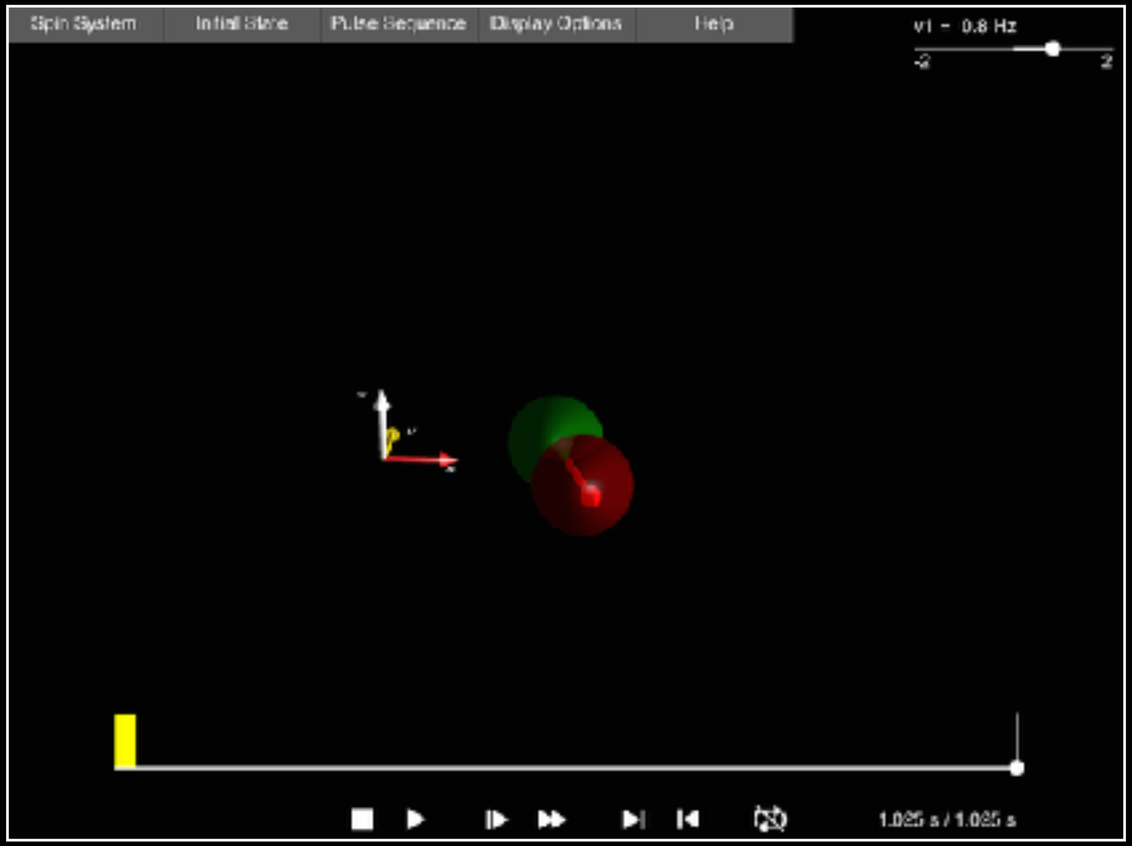




By pressing the play button at the bottom of the screen, you start the simulation of the pulse sequence and immediately see the effect on the screen. The pulse flips the spin by 90° around the y axis from z to x. During the delay, the spin rotates (precesses) around the z axis. The current time point is indicated by a white circle and a vertical white line.

At the end of the sequence, the spin points along the x axis. As described in more detail in the tutorial, the buttons at the bottom of the screen allow you to interactively control the simulation. For example, you can slow down or speed up the simulation, or run the simulation in a loop. After stopping or pausing the simulation, you can move the current time point also by dragging it with your finger.

Example 1: Excitation and Precession of a Single Spin (F)



Note that you can also change the offset frequency (i.e. the rotation frequency during the delay) interactively while the simulation is running and you immediately see the effect of the parameter change. For example, for v1=0.8 Hz, the magnetization vector at the end of the delay does not point along the x axis as was the case for v1=1 Hz.

Discussion: In this simple example, you learned how to define a spin system, the spin system parameters, the initial state, the pulse sequence and how to run and control the simulation. As we considered a single, uncoupled spin, the spin dynamics can be completely described by the well-known vector representation. In addition to the “magnetization vector”, the corresponding single-spin *droplet* (consisting of a red and green sphere) of the DROPS representation was displayed. Although this did not provide any additional information in this case, it is interesting to note that at all times, the magnetization vector is parallel to the corresponding *droplet*, i.e. to the axis formed by the centers of the green and red spheres. Hence, for the simple case of an uncoupled spin 1/2, the vector picture can be viewed as a special case of the DROPS representation. However, in contrast to the vector picture, the DROPS representation is not limited to uncoupled spins.

Example 1: Excitation and Precession of a Single Spin (G)

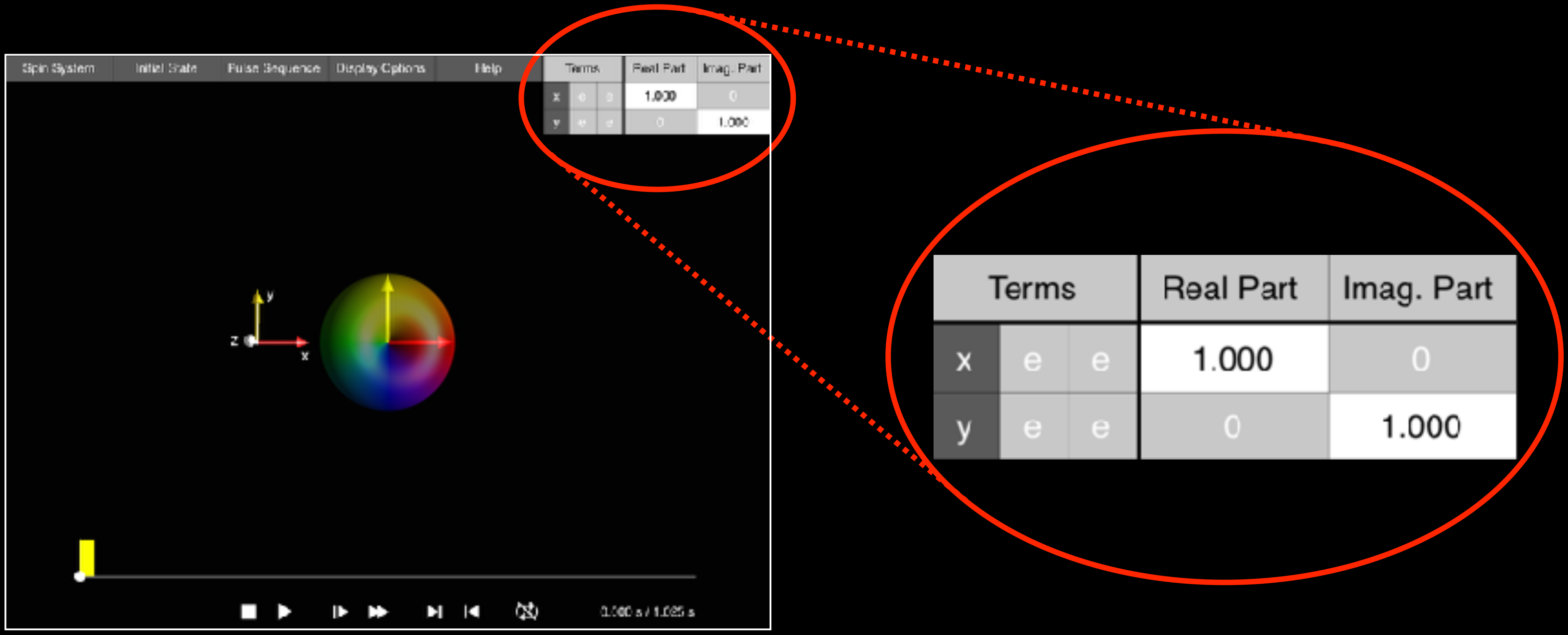
Suggestions for further exploration:

Predict the effect of the pulse sequence for different initial states and check your prediction by running the simulation.
Examples:

(I) Observe the effect of the pulse sequence for the initial state I1x rather than I1z.
(II) Observe the effect of the pulse sequence for the initial state I1y.

What is the effect of the phase and/or flip angle of the excitation first pulse is modified? Selecting *Display Options > List/Edit Seq.* provides the *Sequence List*, which in this case consists of two sequence elements: (1) The pulse 90°_y and (2) the *Delay 1s*. If you double tap on 90°_y, a sub menu opens in which you can change the flip angle and the phase of the pulse. In most cases, the pulses of interest will be 90° or 180° pulses, which can be chosen directly. If you would like to change the 90°_y pulse e.g. to a 45°_y pulse, select *Other Pulse* and enter the desired flip angle in the displayed number pad.

Example 2: Rotation of I^+ Around the z Axis (A)

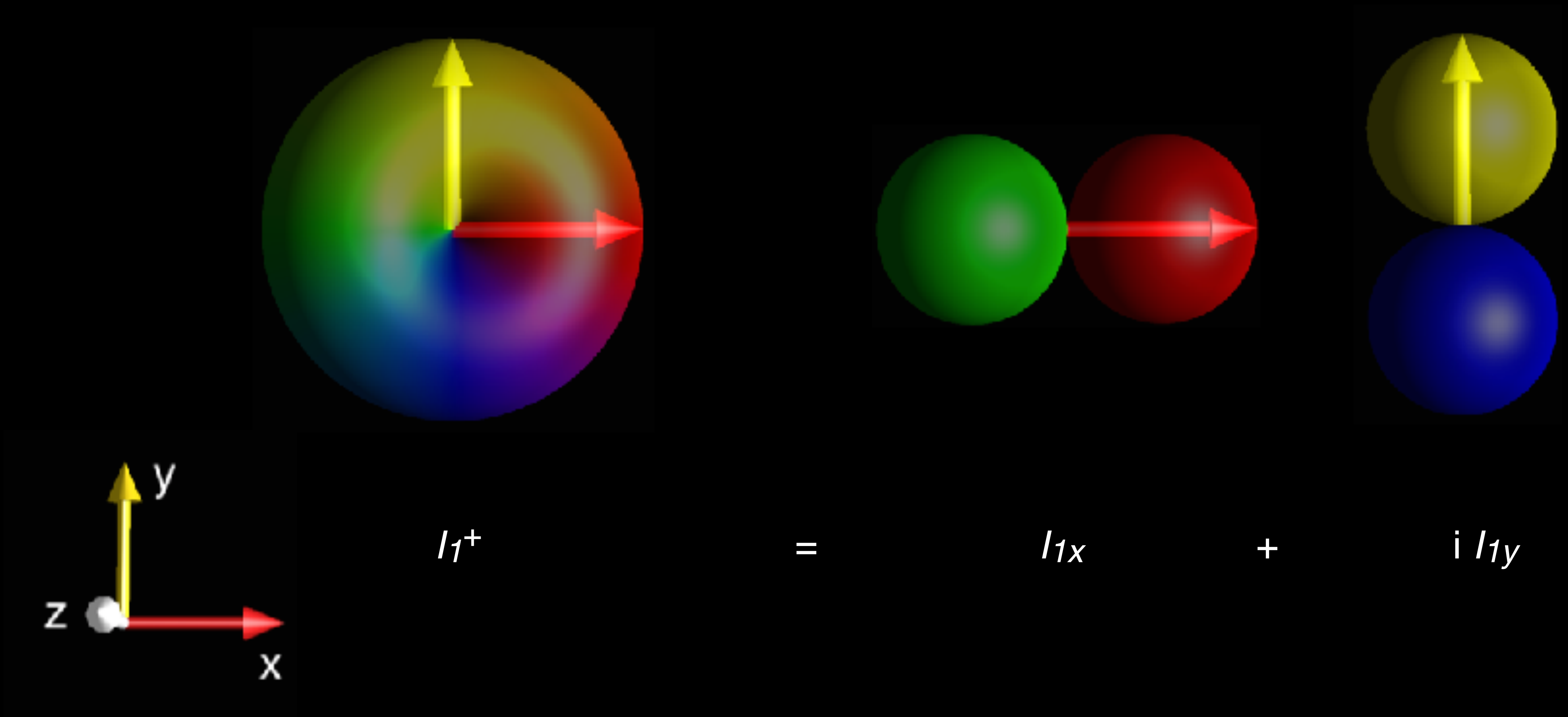


Terms			Real Part	Imag. Part
x	e	e	1.000	0
y	e	e	0	1.000

In this example, we use the *SpinDrops* app to visualize the droplet of the +1-quantum coherence term $I_1^+ = I_{1x} + i\, I_{1y}$ and to see its evolution under z rotations. Choose *Spin System > 1 Spin* and select *Initial State > I1(+)*. To see the corresponding Cartesian product operators, select *Display Options > List Prod. Ops.*

The left column of the list indicates the operator terms using the short-hand three-letter code (see *Help > Tutorial*). On the right, the real and imaginary parts of the corresponding coefficients are displayed, which in general can be complex.

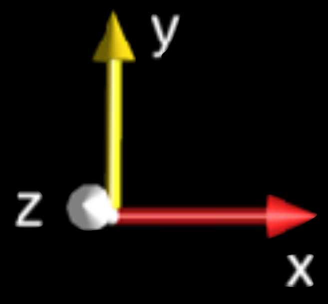
Example 2: Rotation of I^+ Around the z Axis (B)

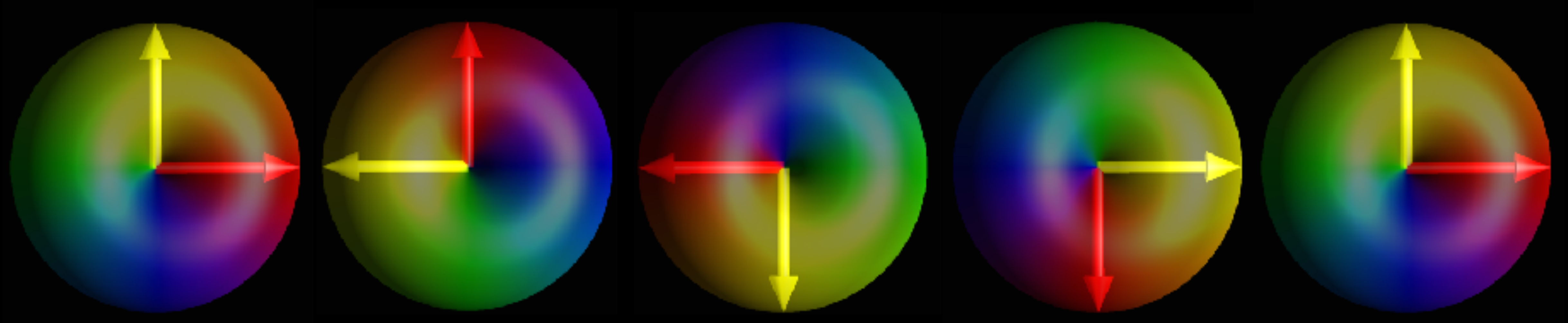


In the vector picture, the state $I_1^+ = I_{1x} + i\, I_{1y}$ is represented by two vectors: A real vector (red) pointing along the *x* axis and an imaginary vector (yellow) pointing along the *y* axis.

The corresponding droplet is a combination of the droplet for the operator I_{1x} (consisting of a red and a green sphere) and the droplet for the operator iI_{1y} (consisting of a yellow and blue sphere).

Example 2: Rotation of I^+ Around the z Axis (C)





0°_z 90°_z 180°_z 270°_z 360°_z

Select *Pulse Sequence > Rotation > z Rotation > 360°(z)* and touch the play button (▶) to start the rotation. You can slow down or speed up the rotation by touching the corresponding control buttons (|▶ or ⏩).

If the repeat mode is off (indicated by ~~🔁~~), you can turn it on by touching the ~~🔁~~ symbol. (The 🔁 symbol indicates that the repeat mode is on). This will result in a continuous rotation of the droplet around the z axis.

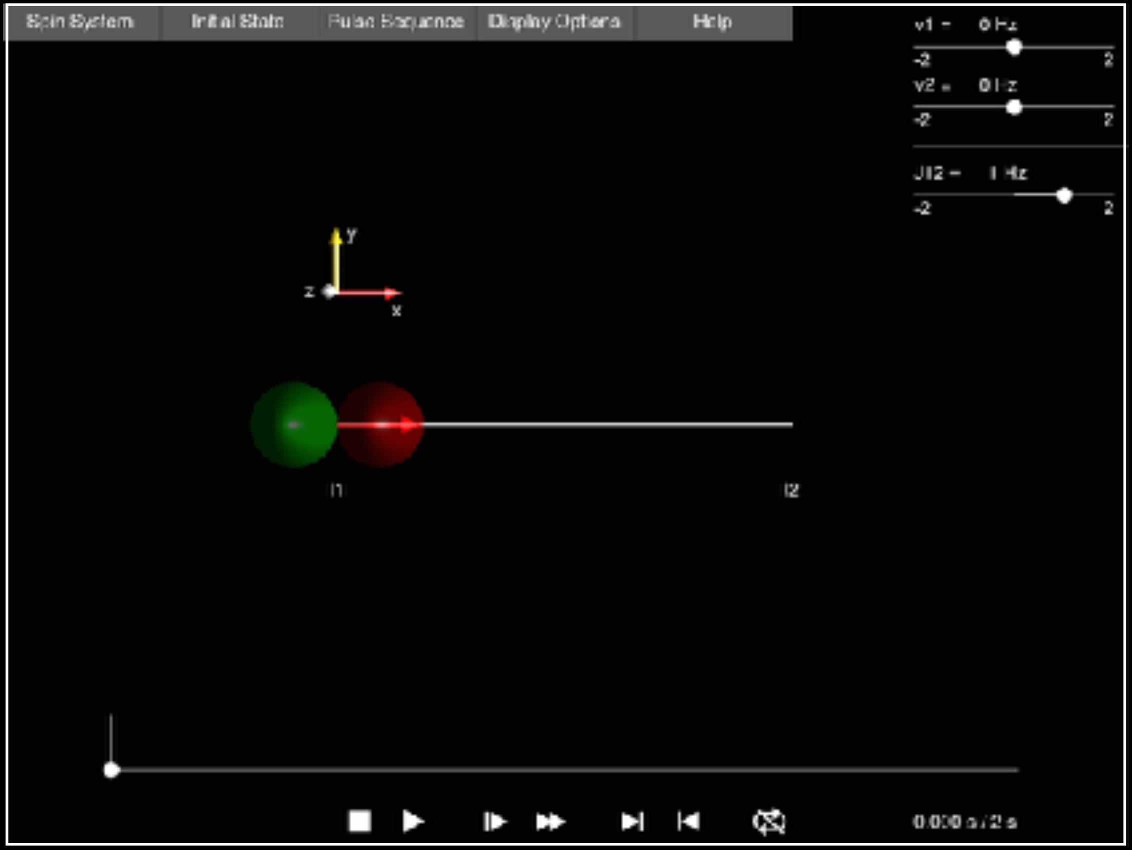
Example 2: Rotation of I^+ Around the z Axis (D)

Suggestions for further exploration:

Observe the effect of the z rotation for different initial states, such as I_1^- or I_{1x}.

Apply different rotations (e.g. around the x or y axis) using pulses.

Example 3: Weak Coupling Evolution in a Two-Spin System (A)



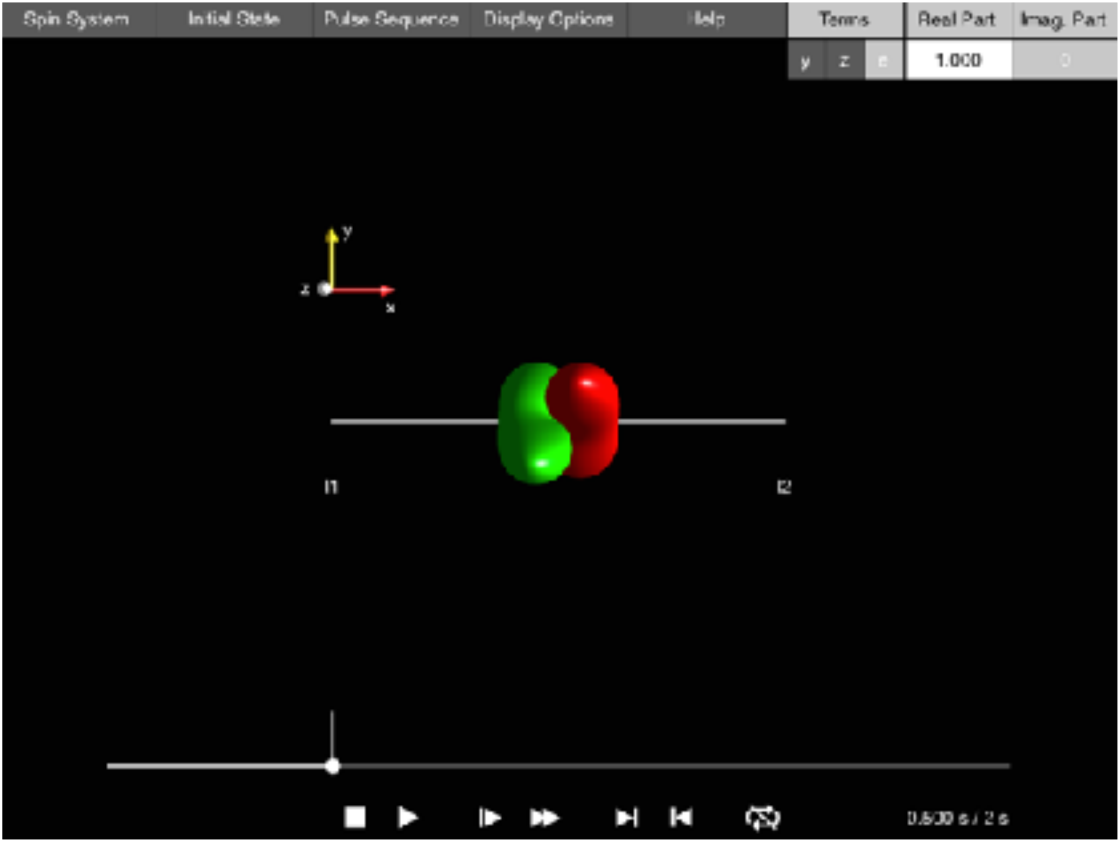
v1 = 0 Hz

v2 = 0 Hz

J12 = 1 Hz

0.000 s / 2 s

Select *Spin System > Two Spins* and choose I_{1x} as the initial state by selecting *Initial State > I1x*. Select *Pulse Sequence > Delay T > T =* 1 *s*. In *Display Options > List Sequence* double tap the delay and set it to 2 s. Change the spin system parameters to v1=0 Hz, v2=0Hz, J12=1 Hz (if the parameter sliders are not visible at the top right of the screen, select *Spin System > Parameters*). Touch the play button to run the simulation.



Terms			Real Part	Imag. Part
y	z	e	1.000	0

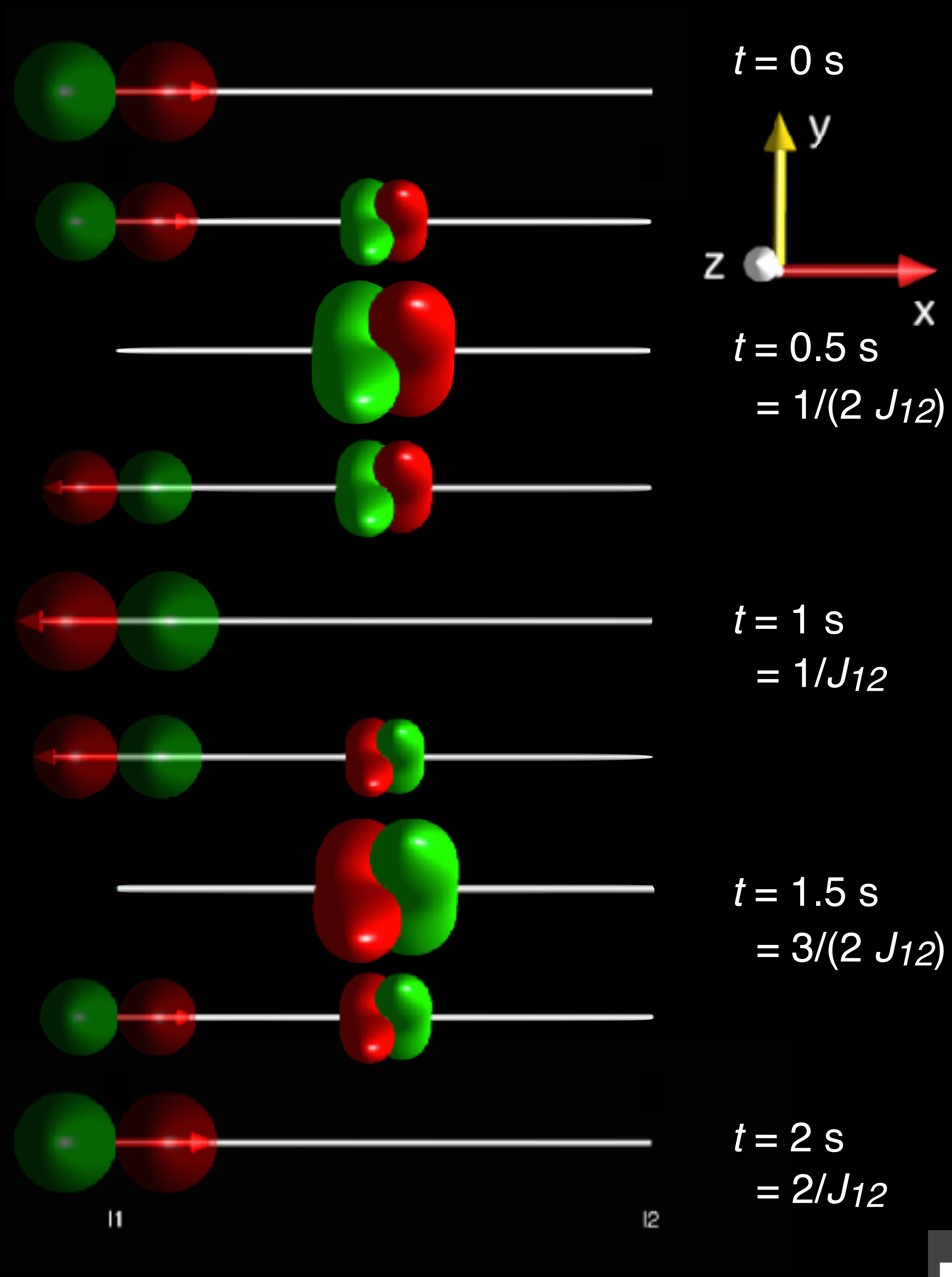
0.500 s / 2 s

Initially, the droplet representing the linear spin operators of *I1* shrinks and a new droplet emerges between *I1* and *I2,* corresponding to the antiphase operator $2I_{1y}I_{2z}$ (confirm using *Display Options > List Prod. Ops.* or using the right-hand rule). After 0.5 seconds (corresponding to $1/(2\ J_{12})$, the *I1* spin droplet has completely vanished and the bilinear {*I1*,*I2*} droplet has reached its maximum size.

Example 3: Weak Coupling Evolution in a Two-Spin System (B)

After 1 second (corresponding to $1/J_{12}$), the $\{I_1,I_2\}$ droplet vanishes and the I_1 droplet reaches its maximum size again. However, note that the sign of the $I1$ droplet (and of the magnetization vector) is inverted compared to the initial state at $t = 0$ s. After 2 seconds (corresponding to $2/J_{12}$), the initial state I_{1x} is reproduced. If the simulation is set to repeat mode, this will result in a continuous oscillation between the two droplets.

This simulation visualizes the well-known evolution of I_{1x} in the presence of a J coupling (in the weak coupling limit), which is given by $I_{1x} \cos(\pi J_{12} t) + 2I_{1y}I_{2z} \sin(\pi J_{12} t)$. For $J_{12} =$ 1 Hz and $t = 0.5$ s, the argument $(\pi J_{12} t) = \pi/2$, i.e. the state is given by $I_{1x} \cos(\pi/2) + 2I_{1y}I_{2z} \sin(\pi/2) = 2I_{1y}I_{2z}$. For $t = 1$ s, 1.5 s, and 2 s, the state is $-I_{1x}$, $-2I_{1y}I_{2z}$, and I_{1x}, respectively.



Example 3: Weak Coupling Evolution in a Two-Spin System (C)

Suggestions for further exploration:

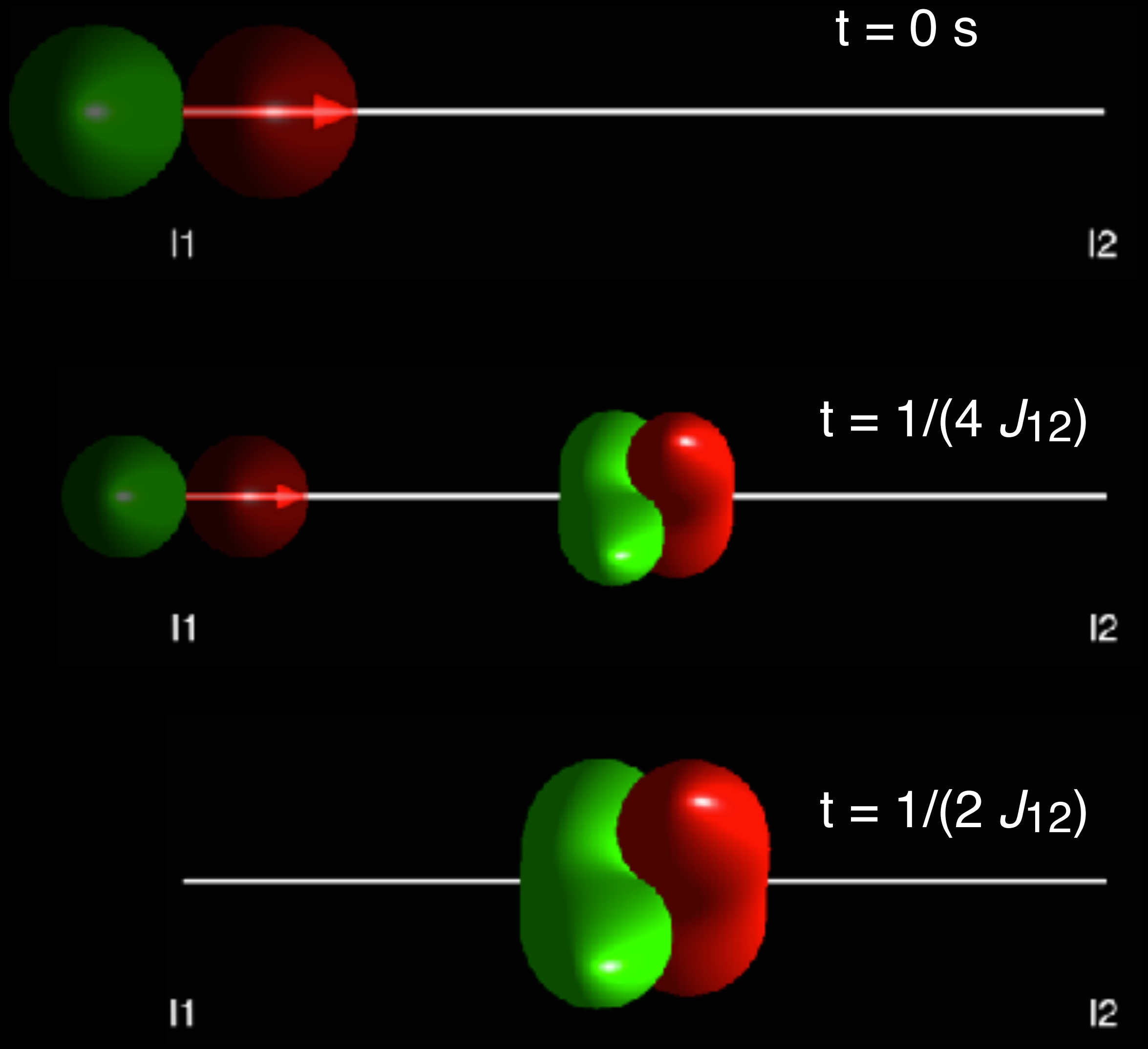
(I) What happens if the offset frequency v1 is set to non-zero values?
(II) What is the effect if the offset frequency v2 is set to non-zero values?
(III) What happens if the initial state is I_{1z}?

Example 4: Refocusing of Offset and Coupling Effects (A)

In this example, we illustrate the effect of 180° pulses on the evolution of a two-spin system. Select *Spin System > 2 Spins* and set J_{12} = 1 Hz using the parameter slider (*Spin System > Parameters*).

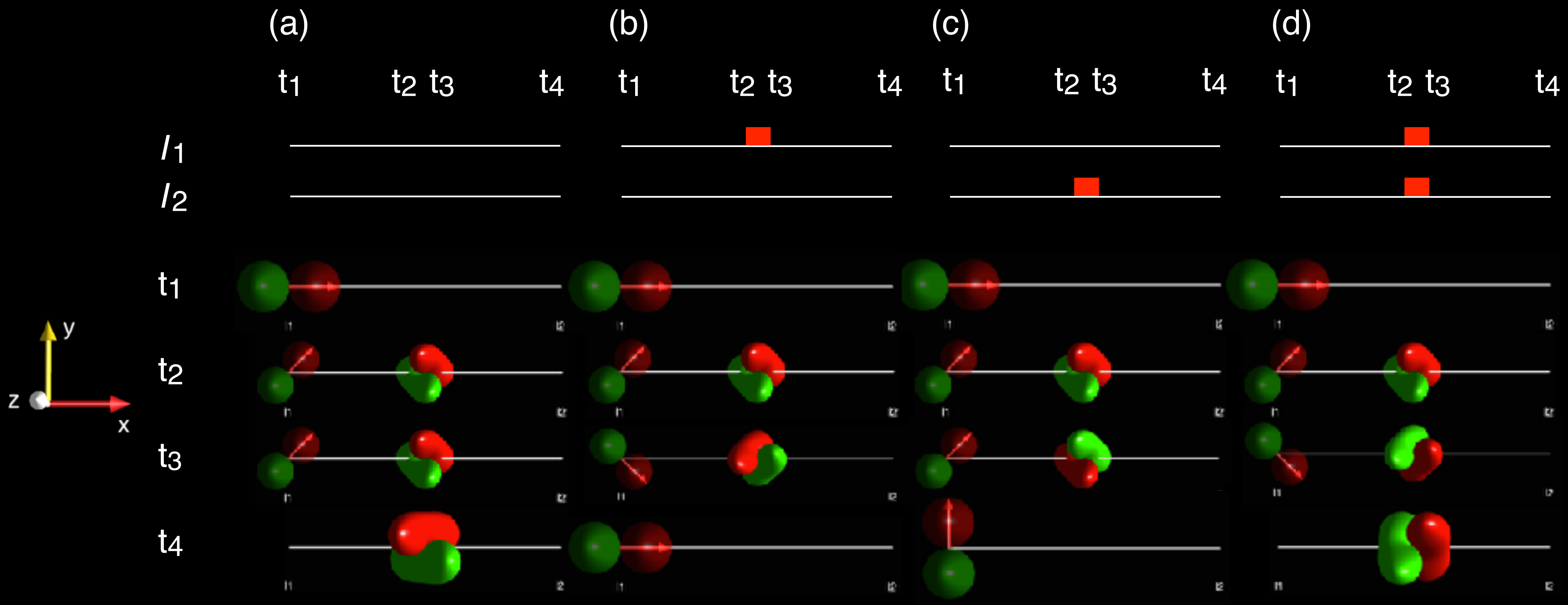
We consider the evolution of the initial state I_{1x} (select *Initial State > I1x*) during a delay T = 1/(2 J_{12}) = 0.5 s (select *Pulse Sequence > Delay T > T=1/(2·J12)*).

The Figure on the right shows the DROPS visualization of the product operator terms at t = 0 s, at t = 1/(4 J_{12}) = 0.25 s, and at t = 1/(4 J_{12}) = 0.5 s for the case where both offset frequencies are zero ($\nu_1 = \nu_2 = 0$ Hz).



In this case, initial x magnetization of the first spin (I_{1x}) evolves under the weak coupling Hamiltonian during the delay T = 1/(2 J_{12}) completely to the anti-phase operator $2I_{1y}I_{2z}$. In the following, we simulate the resulting final state without and with additional 180° pulses in the center of the delay T, assuming a non-zero offset frequency of the first spin (ν_1 = 0.5 Hz).

Example 4: Refocusing of Offset and Coupling Effects (B)

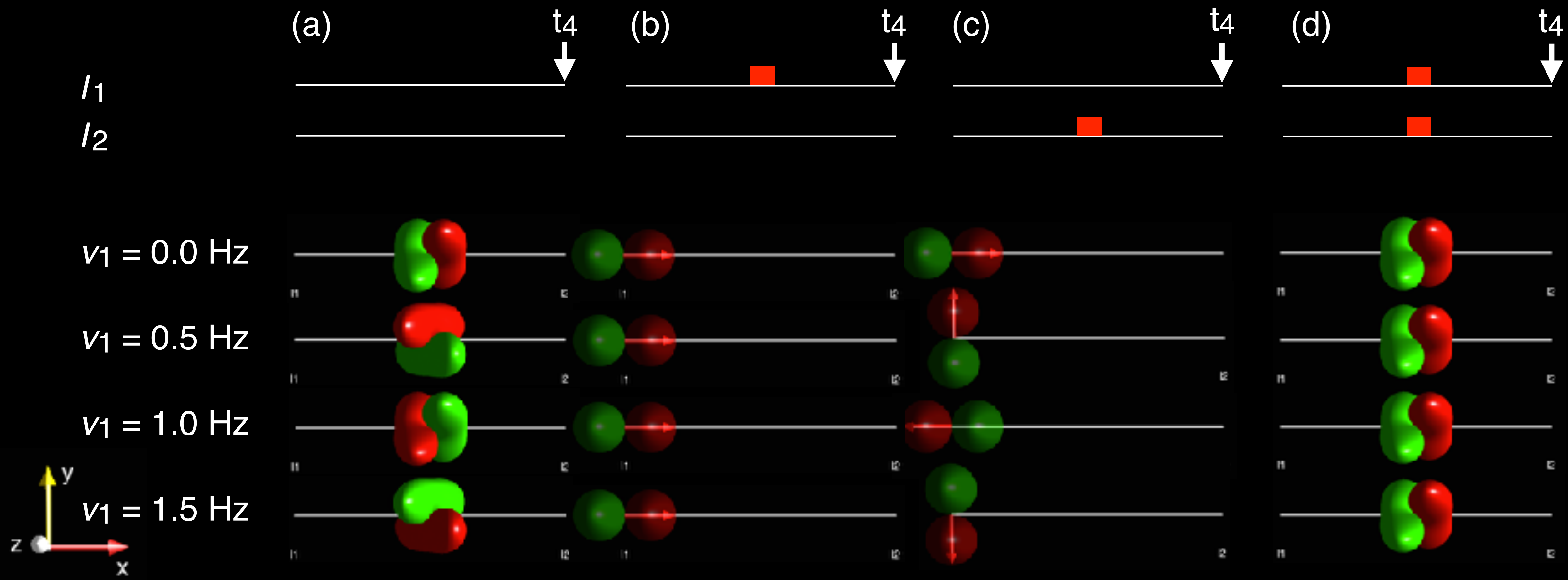


For $\nu_1 = 0.5$ Hz and $J_{12} = 1$ Hz, simulations are shown for $t_1 = 0$ s, $t_2 = T/2 = 1/(4 J_{12}) = 0.25$ s, $t_3 = t_2$ (assuming a negligible duration of the180° pulses) and $t_4 = T = 1/(2 J_{12}) = 0.5$ s. I_{1x} evolves

(a) to $-2I_{1x}I_{2z}$ in the absence of pulses during the delay T,
(b) to I_{1x} if a spin I_1-selective 180°x pulse is irradiated at T/2,
(c) to I_{1y} if a spin I_2-selective 180°x pulse is irradiated at T/2,
(d) to $2I_{1y}I_{2z}$ if I_1- and I_2-selective 180°x pulses are irradiated at T/2.

Example 4: Refocusing of Offset and Coupling Effects (C)

The results of the previous page reflect the well-known fact that in case (a), offset and coupling terms of the Hamiltonian are active. In (b), the effect of the coupling and of the offset ν_1 are refocused. In (c), the effect of the coupling and of the offset ν_2 are refocused but ν_1 is active. In (d), the simultaneously irradiated I_1- and I_2-selective 180°x pulses at T/2 (corresponding to a non-selective 180°x pulse for the two-spin system) refocus frequency-offset effects but the coupling evolution is active. For the initial state I_{1x}, this is confirmed by the resulting final state of the system at $t_4 = T = 1/(2\,J_{12}) = 0.5$ s for different offsets ν_1 of 0 Hz, 0.5 Hz, 1 Hz and 1.5 Hz.



Example 4: Refocusing of Offset and Coupling Effects (D)

Suggestions for further exploration:

Has the offset v_2 of the second spin an effect in the experiment considered in the given example? What if we start with the initial state I_{2x} instead of I_{1x}?

How would the results change if $180°_y$ pulses rather than $180°_x$ pulses would be used in the example?

Explore the effects of selective and non-selective 180° pulses in three-spin systems.

Explain the results of the refocusing experiments using the product operator formalism.

Example 5: Spectral Editing (A)

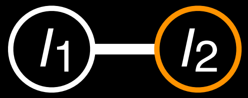
The DEPT experiment (Distortionless Enhancement of Polarization Transfer) makes it possible to distinguish C, CH, CH_2, and CH_3 groups. The ^1H spins are excited and the amplitude and sign of the detected ^{13}C spin depends on the number of attached protons.

The basic pulse sequence of the DEPT experiment has the form

$$90°_x(H) - T - 180°_x(H), 90°_x(C) - T - \theta_y(H), 180°_x(C) - T$$

where the flip angle θ of the editing ^1H pulse is 45°, 90° or 135° and the delay T is $1/(2\ J_{CH})$. The experiment relies on *polarization transfer* and only signal originating from ^1H polarization is detected on the ^{13}C frequency. Hence, the spins of ^{13}C atoms without attached ^1H atoms do not yield any detectable signal. Predicting the ^{13}C signals of CH, CH_2, and CH_3 is less simple.

As up to three spins 1/2 can be considered in the current version of *SpinDrops*, it is possible and instructive to simulate the relative size and sign of of the final ^{13}C magnetization (and hence of the relative size and sign of the corresponding ^{13}C NMR signal) for CH, CH_2 groups. In the following, we will assume that spin I_2 represents a ^{13}C spin and spins I_1 and I_3 represent ^1H spins:

CH system: 

with $J_{12} \neq 0$ and $J_{13} = J_{23} = 0$.

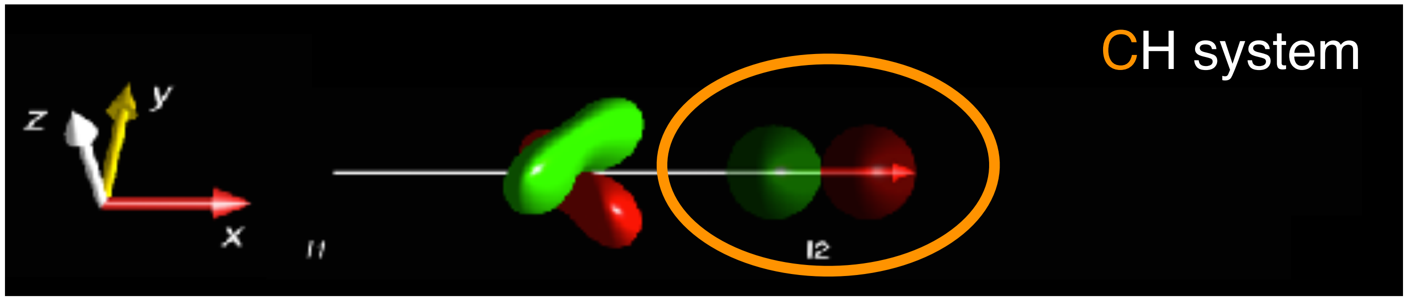
CH_2 system: 

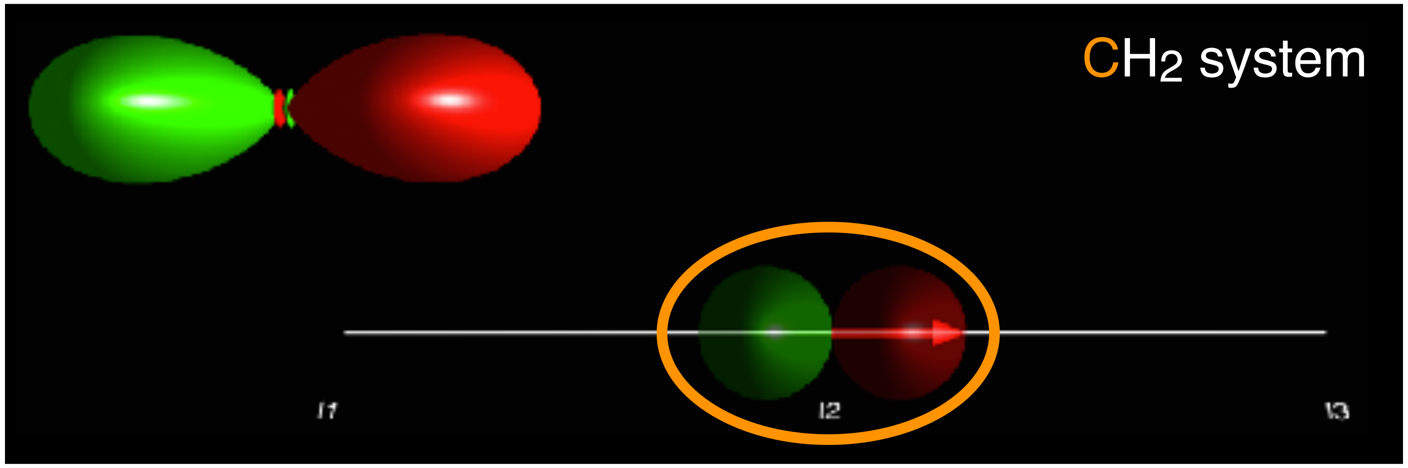
with $J_{12} = J_{23} \neq 0$ and $J_{13} = 0$.

Example 5: Spectral Editing (B): DEPT-45

Selecting *Spin System > 3 Spin Chain* automatically sets $J_{13} = 0$. To simulate the CH system, set J_{12} = 1 Hz and J_{23} = 0 Hz (*Spin System > Parameters*) and define the initial state as I_{1z} (*Initial*
Selecting *Spin System > 3 Spin*
State > I1z). For the CH2 system, set J_{12} = 1 Hz and J_{23} = 1 Hz and define the initial state as $I_{1z}+I_{3z}$ (*Initial State > Edit operator*). Select *Pulse Sequence > Sequence List > Heteronuclear > DEPT-45* and run the simulation.

Note that in both cases the final ~~magnetization vector of spin I_2 is~~ pointing in the positive x direction (orange ellipses).


CH system

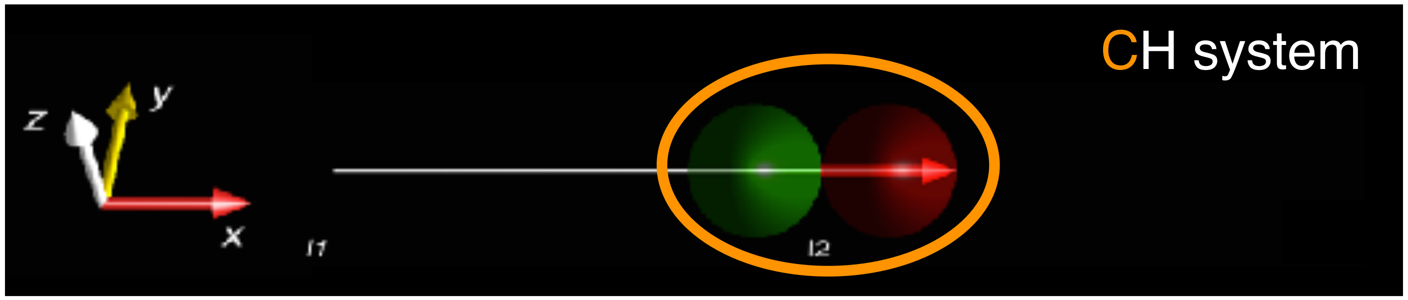

CH2 system

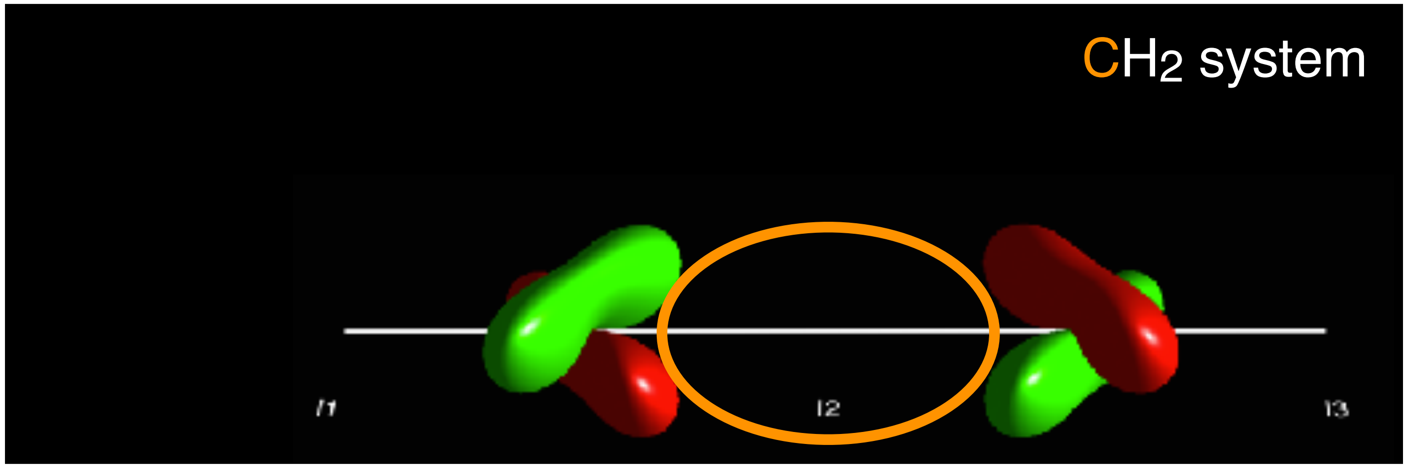

DEPT-45

Example 5: Spectral Editing (C): DEPT-90

Select *Pulse Sequence > Sequence List > Heteronuclear > DEPT-90* and run the simulation. Note that compared to the DEPT-45 sequence shown on the previous page, the flip angle θ of the editing pulse has changed from 45° to 90° (yellow ellipses).

In DEPT-90, the final magnetization vector of spin I_2 is pointing in the positive x direction for CH (orange ellipse). However, for CH_2 the final magnetization vector of spin I_2 is zero (orange ellipse). This results in positive ^{13}C-NMR signals for CH groups but no ^{13}C-NMR signals for CH_2 groups.


CH system

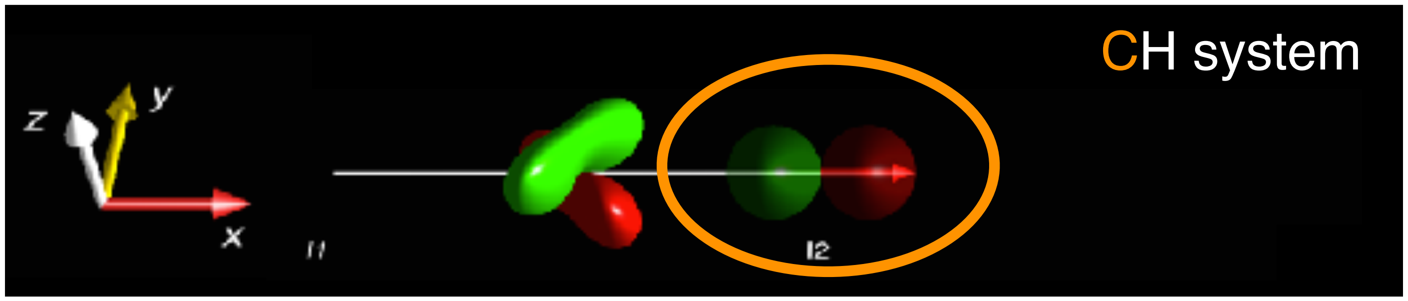

CH_2 system

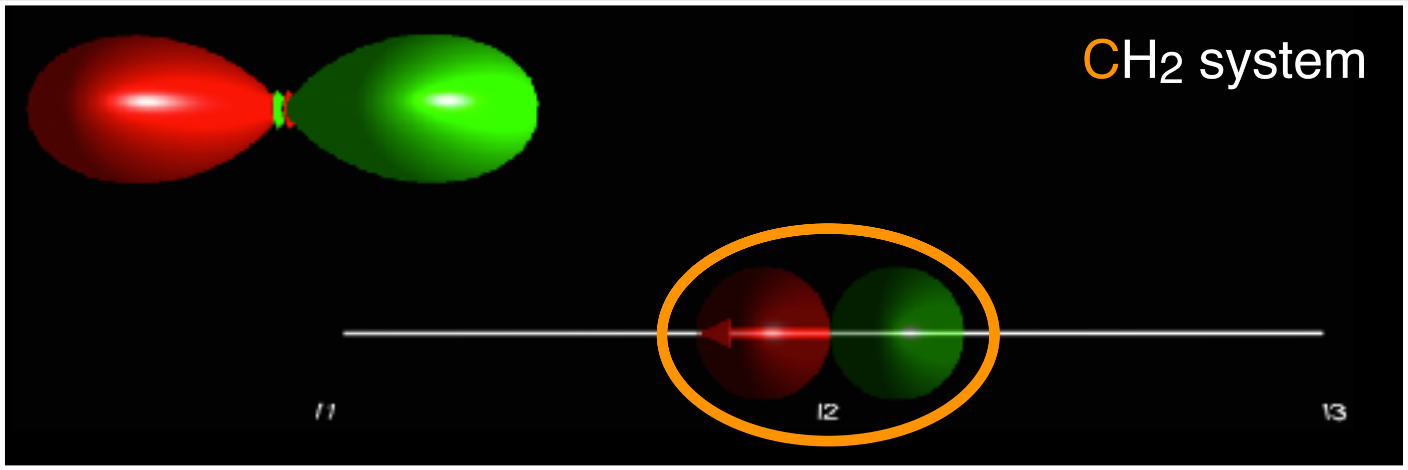

DEPT-90

Example 5: Spectral Editing (D): DEPT-135

Selecting *Pulse Sequence > Sequence List > Heteronuclear > DEPT-135* changes the flip angle θ of the editing pulses to 135° (yellow ellipses).

In this case of DEPT-135, the final magnetization vector of spin *I_2* is pointing in the positive x direction for the CH system, whereas it is pointing in the negative x direction for the CH_2 system (orange ellipses). This results in positive and negative ^{13}C-NMR signals for CH and CH_2 groups, respectively.





Example 5: Spectral Editing (E)

Suggestions for further exploration:

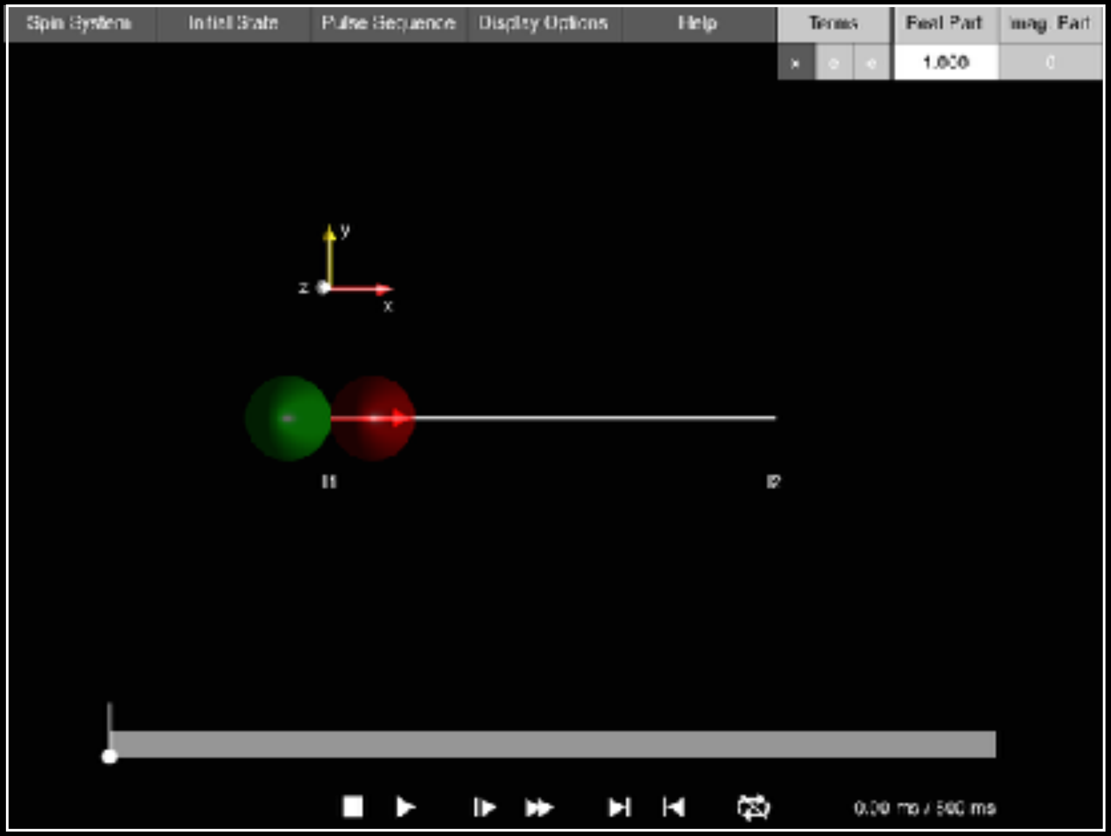
What are the expected relative signal amplitudes for CH and CH_2 groups in DEPT-45, DEPT-90 and DEPT-135? (*Tip*: Remember that you can always display the coefficients of the product operator terms by selecting *Display Options > List Prod. Ops.*)

Does the final DROPS display (and hence the final state of the spin system) depend on the offset frequencies v_1, v_2, v_3?

Which product operator terms are created at the end of DEPT-45, DEPT90, and DEPT-135 in addition to the desired magnetization of spin I_2?

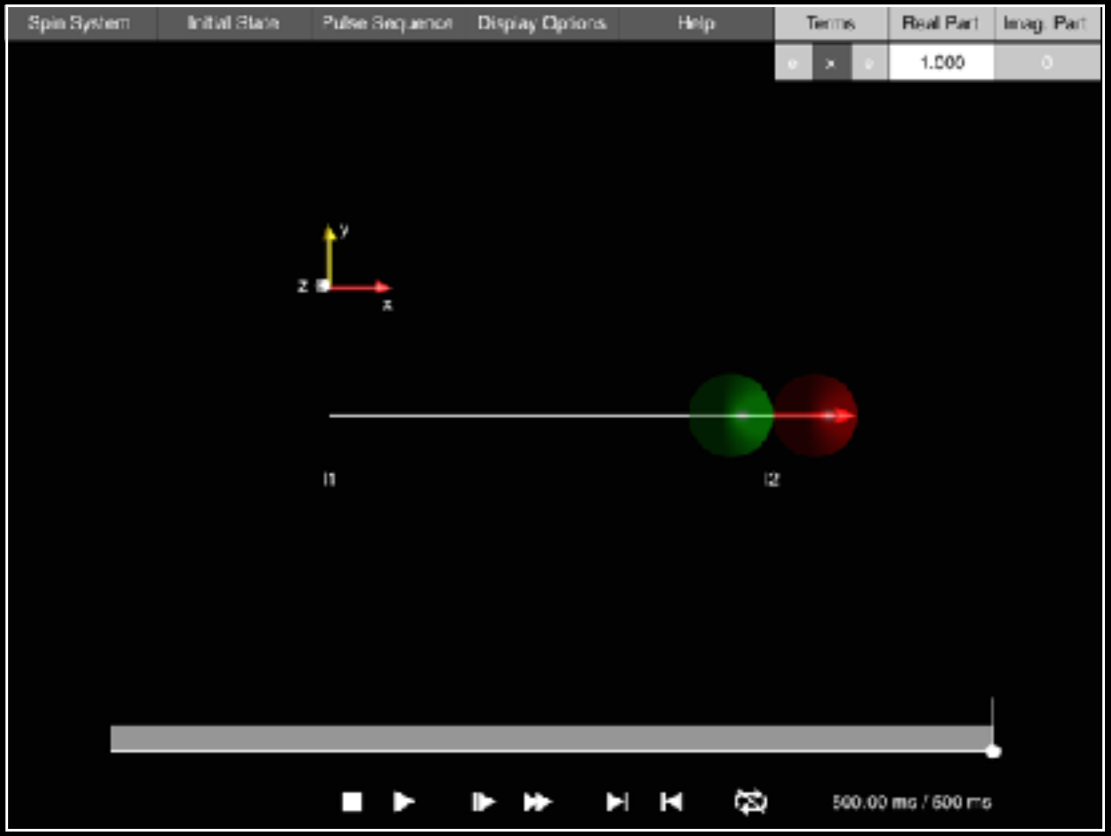
Calculate the effect of the DEPT experiments analytically using the standard product operator formalism and compare the results with the DROPS simulations. What are the expected relative signal amplitudes for CH_3 groups in DEPT-45, DEPT-90 and DEPT-135?

Example 6: TOCSY Transfer in a Two-Spin System (A)



In this example, we explore the transfer of x magnetization in the isotropic mixing period of TOCSY experiments, where isotropic mixing conditions are created by a multiple-pulse sequence.

Select *Spin System > Two Spins* and choose I_{1x} as the initial state by selecting *Initial State > I1x*. Choose the isotropic mixing sequence for two spins by selecting *Pulse Sequence > Sequence List > Homonuclear > Isotropic Mix. 12*.



The isotropic mixing period is indicated by a grey rectangle. Set the coupling J12 to 1 Hz. (Here, the offset frequencies v1 and v2 are irrelevant as they are effectively suppressed by the isotropic mixing sequence.)

Interestingly, after 0.5 seconds, corresponding to $t = 1/(2\ J_{12})$, the initial state I_{1x} has turned completely into I_{2x}, i.e. x magnetization has been fully transferred from the first to the second spin).

Example 6: TOCSY Transfer in a Two-Spin System (B)

Under the isotropic mixing Hamiltonian, the initial state $\rho(0) = I_{1x}$ evolves to

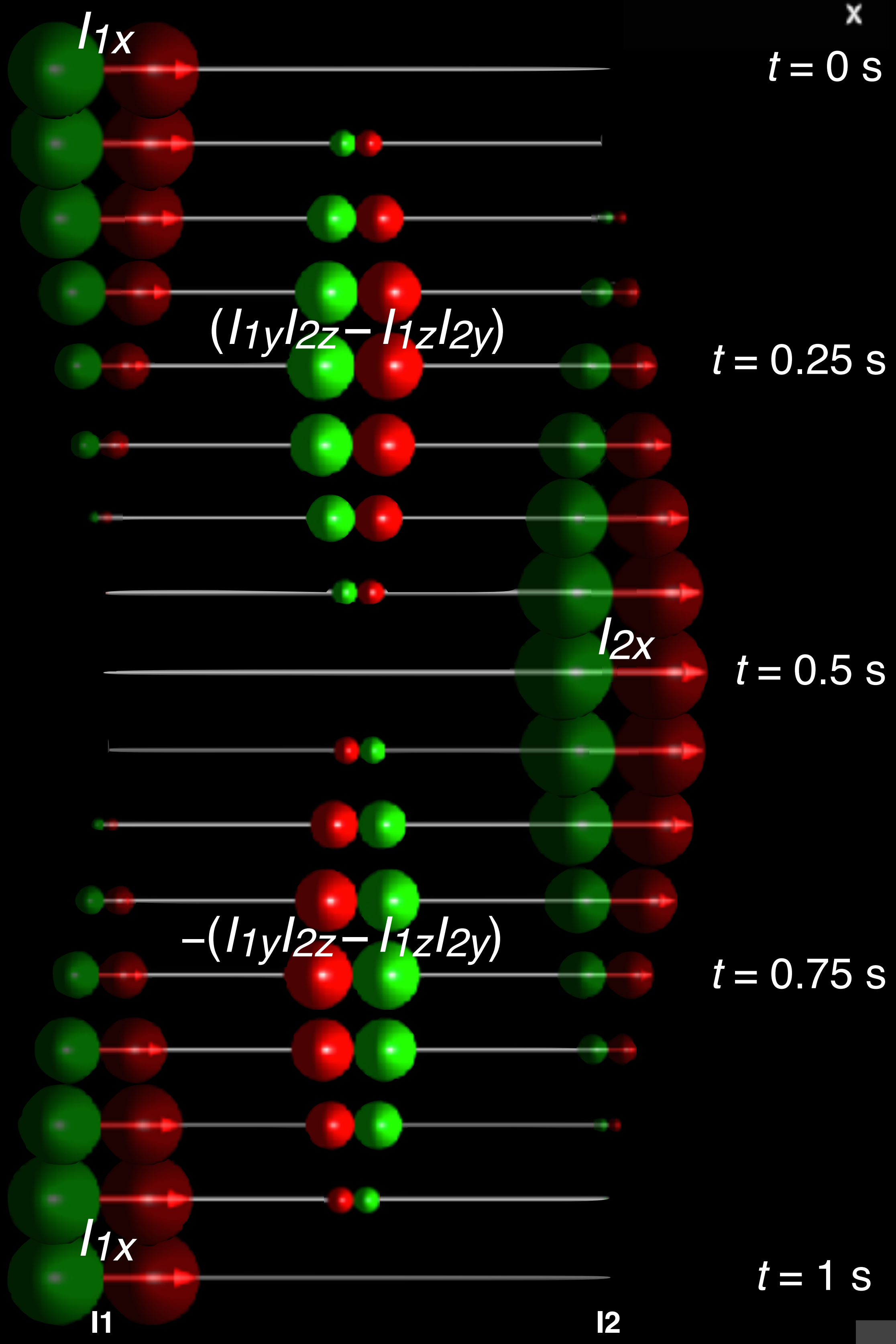
$$\rho(t) = I_{1x}\cos^2(\pi J_{12}\, t) + (2I_{1y}I_{2z} - 2I_{1z}I_{2y})\cos(\pi J_{12}\, t)\sin(\pi J_{12} t) + I_{2x}\sin^2(\pi J_{12}\, t).$$

This is depicted on the right, where the isotropic mixing period was extended to 1 s (by selecting *Display Options > List/Edit Seq.*, double tapping *Hiso12*, and changing *0.5/J12* to *1/J12*.)

For $t = 1/(4J_{12})$ (corresponding to $t = 0.25$ s for $J_{12} = 1$ Hz), the argument $(\pi J_{12}\, t) = \pi J_{12}/(4J_{12}) = \pi/4$ and $\cos(\pi J_{12}\, t) = \sin(\pi J_{12}\, t) = 1/\sqrt{2}$. Hence the state is $0.5\ I_{1x} + (I_{1y}I_{2z} - I_{1z}I_{2y}) + 0.5\ I_{2x}$ and the bilinear droplet located between I1 and I2 reaches its maximum value.

For $t = 1/(2J_{12}) = 0.5$ s, $(\pi J_{12}\, t) = \pi J_{12}/(2J_{12}) = \pi/2$ and $\cos(\pi J_{12}\, t) = 0$, $\sin(\pi J_{12}\, t) = 1$. Hence, the state is I_{2x}, i.e. the initial x magnetization has been fully transferred from spin I_1 to spin I_2.

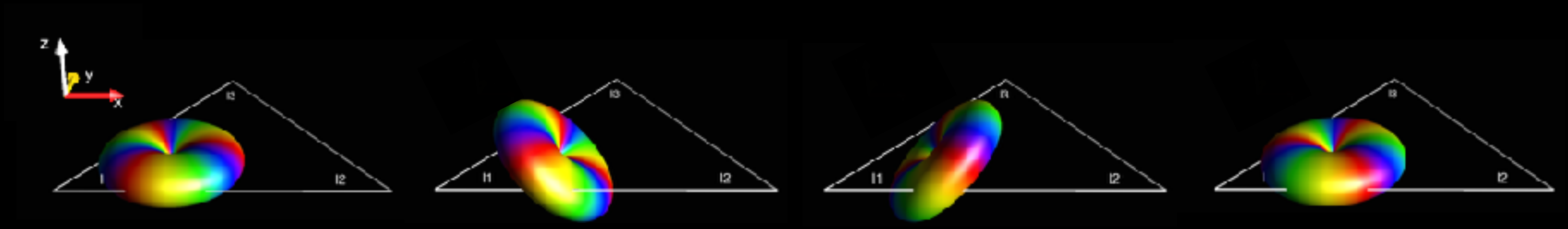
For $t = 1/J_{12} = 1$ s, the state is again I_{1x} and the cycle starts anew.



Example 7: Inversion of Multiple-Quantum Coherence (A)

In the standard *SpinDrops* representation, a non-selective 180y° pulse simply rotates the droplets by 180° around the y axis. This is illustrated here for the initial operator $I_1^+ I_2^+ I_3^+$ (select *Initial State > MQ (+/- ops) > 3Q(I1,I2,I3) > 2*I1(+)*I2(+)*I3(+)*).

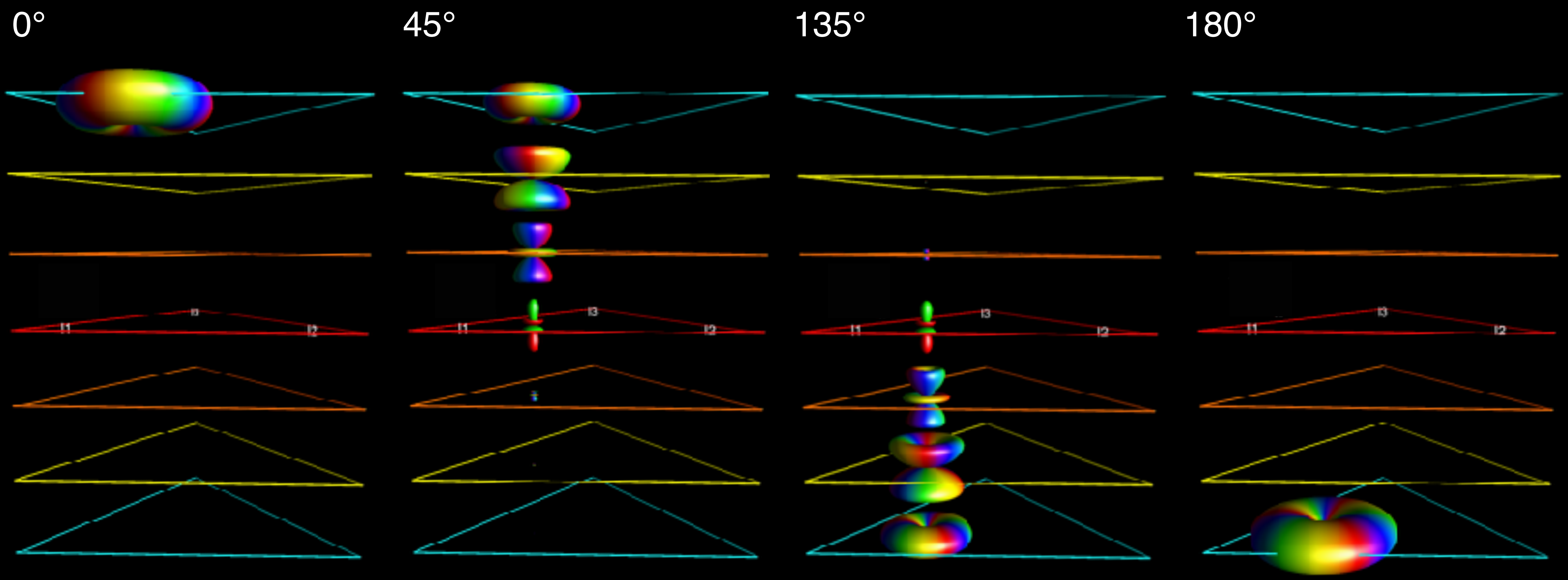
In addition to the initial orientation of the droplet, the snapshots show its orientations after rotations of 45°, 135°, and 180° around the y axis.



The fact that this operation also inverts the coherence order from *p*=+3 to *p*=–3 can be inferred from the direction of the rainbow colors of the initial and final droplet orientations. However, this can be seen more directly by separating the droplet according to coherence order *p*.

Example 7: Inversion of Multiple-Quantum Coherence (B)

On the previous page, „*Standard Plane*“ display mode was selected. To separate the droplets according to coherence order *p*, choose *Display Options > Separation > Coh. Order p*. In this display mode, the change of coherence order from *p*=+3 to *p*=–3 (via all the intermediate coherence orders) can be clearly followed. In *Coh. Order p* display mode, the droplets are arranged in planes with coherence order *p*=3 at the top and *p*=–3 at the bottom, as explained in *Help > Tutorial > DROPS Display*. The red plane in the center corresponds to *p*=0.



Example 7: Inversion of Multiple-Quantum Coherence (C)

Suggestions for further exploration:

Study the effect of pulses and delays on various initial states of pure or mixed coherence orders.

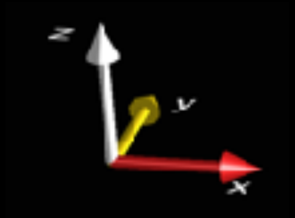
Test the different display modes with droplet separations based on coherence order *p*, the absolute value of coherence order $|p|$ and/or tensor rank *j*.

Challenges

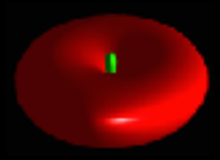
Explore how to define desired states

Challenge 1:

Create the following *droplets* using the menu *Initial State > MQ(x/y ops.)*

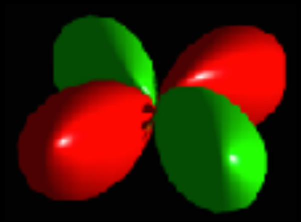


(a)



(b)

(c)

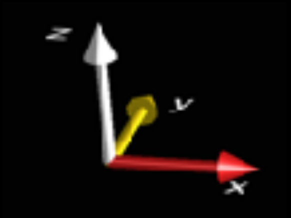


(d)

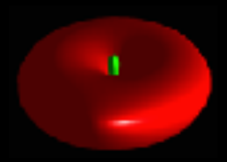
Explore how to define desired states

Challenge 1:

Create the following *droplets* using the menu *Initial State > MQ(x/y ops.)*

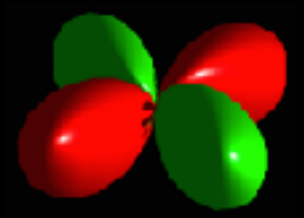


(a)



(b)

(c)



(d)

Solution:

(a) *0Q(I1,I2) > 0Qx(I1,I2)*

(b) *1Q(I1,I2) > 2*I1z*I2y*

(c) *2Q(I1,I2) > 2Qy(I1,I2)*

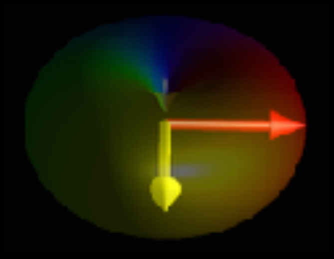
(d) *3Q(I1,I2,I3) > 2*3Qx(I1,I2,I3)*

Explore how to define desired states

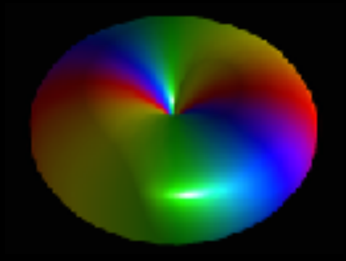
Challenge 2:

Create the following *droplets* using the menu *Initial State > MQ(+/– ops.)*

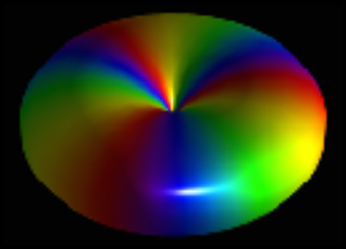
(a)



(b)



(c)

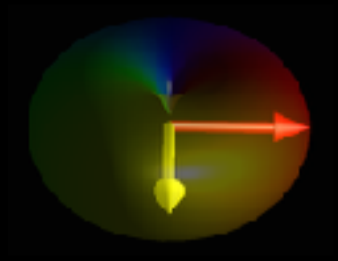


Explore how to define desired states

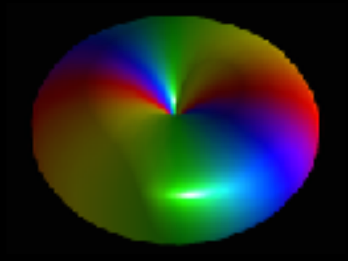
Challenge 2:

Create the following *droplets* using the menu *Initial State > MQ(+/– ops.)*

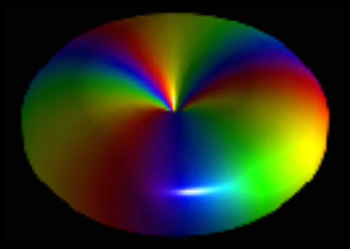
(a)



(b)



(c)



Solution:

(a) *1Q(I1) > I1(–)* (b) *2Q(I1,I2) > I1(+)*I2(+)* (c) *3Q(I1,I2,I3) > 2*I1(-)*I2(-)*I3(-)*

Explore how to define desired states

Challenge 3:

Create the following states using the menu *Initial State > MQ(+/– ops.)*

(a) $I_1^+ I_2^-$

(b) $I_1^- I_2^+$

(c) $2I_1^+ I_{2z}$

Explore how to define desired states

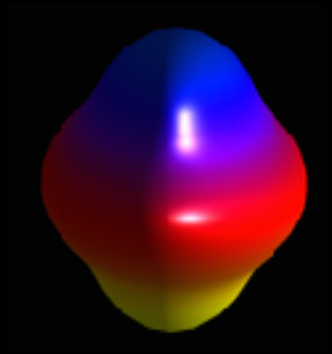
Challenge 3:

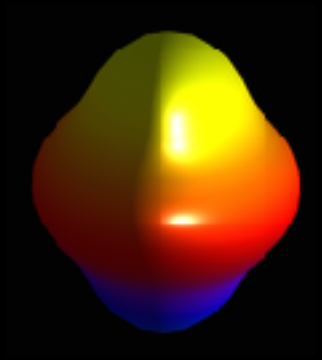
Create the following states using the menu _Initial State > MQ(+/– ops.)_

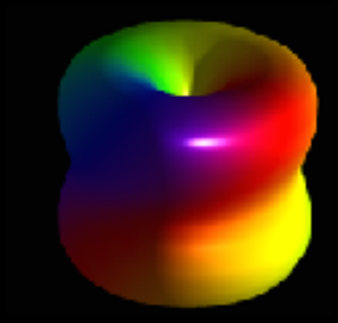
(a) $I_1^+ I_2^-$ (b) $I_1^- I_2^+$ (c) $2 I_1^+ I_{2z}$

Solution:

(a) _0Q(I1,I2) > I1(+)*I2(-)_ (b) _0Q(I1,I2) > I1(-)*I2(+)_ (c) _1Q(I1,I2) > 2*I1(+)*I2z_







Explore how to interpret droplets

Challenge 4:

Using the menu *Initial State > MQ(x/y ops.)* > 2Q(I1,I2), create the operator *2Qx(I1,I2)* and determine how it can be expressed as a linear combination of Cartesian product operators.

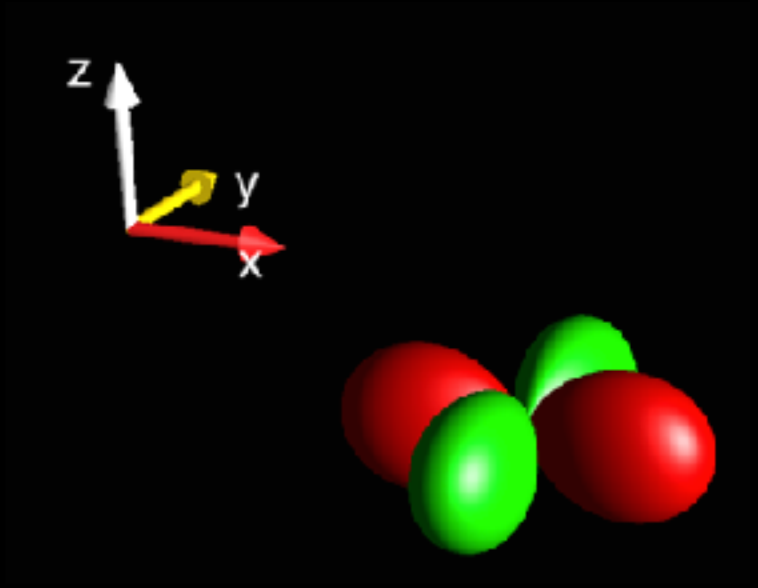
Explore how to interpret droplets

Challenge 4:

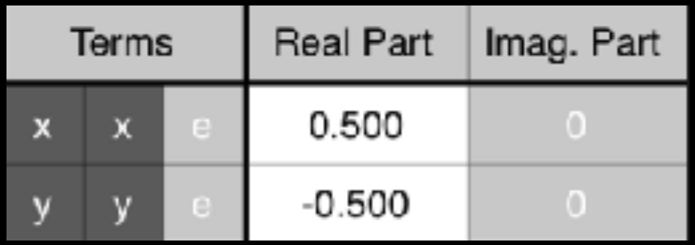
Using the menu *Initial State > MQ(x/y ops.)* > 2Q(I1,I2), create the operator *2Qx(I1,I2)* and determine how it can be expressed as a linear combination of Cartesian product operators.

Solution:

The double-quantum x operator involving spins I1 and I2 corresponds to the following droplet:



Selecting in the menu *Display Options > List Prod. Ops.*, the following terms will be displayed in the shorthand notation for Cartesian operators as shown on the right.



Terms			Real Part	Imag. Part
x	x	e	0.500	0
y	y	e	-0.500	0

Hence, *"2Qx(I1,I2)"* $= 0.5\,(2\,I_{1x}\,I_{2x}) - 0.5\,(2\,I_{1y}\,I_{2y}) = I_{1x}\,I_{2x} - I_{1y}\,I_{2y}$.

Explore how to interpret droplets

Challenge 5:

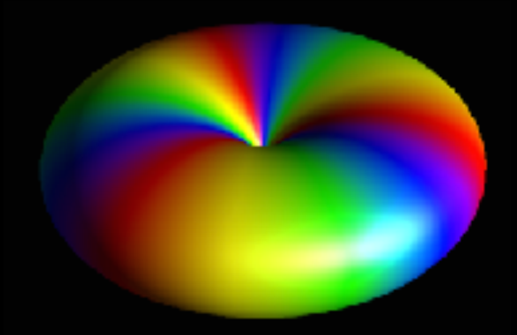
Using the menu *Initial State > MQ(+/– ops.)* > 3Q(I1,I2,I3), create the operator *2*I1(+)*I2(+)*I3(+)* and determine how it can be expressed as a linear combination of Cartesian product operators.

Explore how to interpret droplets

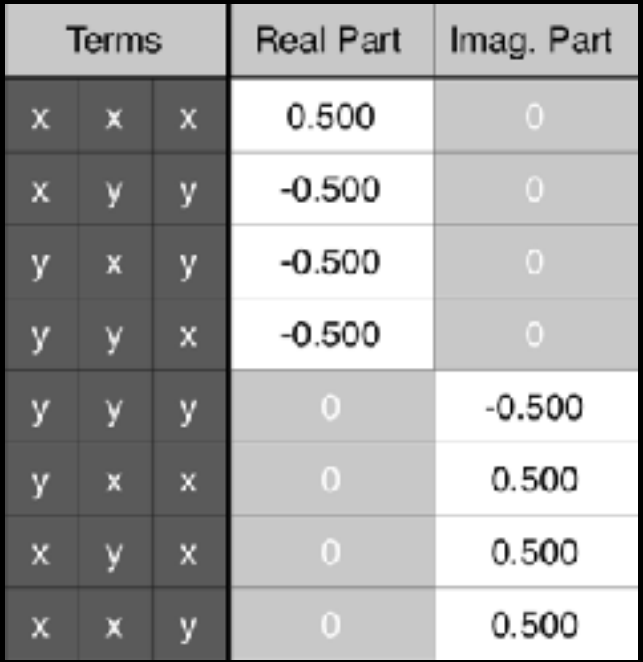
Challenge 5:

Using the menu *Initial State > MQ(+/– ops.)* > 3Q(I1,I2,I3), create the operator *2*I1(+)*I2(+)*I3(+)* and determine how it can be expressed as a linear combination of Cartesian product operators.

Solution: The +3-quantum operator $2\, I_1^+ I_2^+ I_3^+$ corresponds to the following droplet:



Selecting in the menu *Display Options > List Prod. Ops.*, the following terms will be displayed in the shorthand notation for Cartesian operators as shown on the right.



Terms			Real Part	Imag. Part
x	x	x	0.500	0
x	y	y	-0.500	0
y	x	y	-0.500	0
y	y	x	-0.500	0
y	y	y	0	-0.500
y	x	x	0	0.500
x	y	x	0	0.500
x	x	y	0	0.500

Hence,
$$
\begin{aligned}
2\, I_1^+ I_2^+ I_3^+ = {} & 0.5\,(4I_{1x}I_{2x}I_{3x}) \;-\; 0.5\,(4I_{1x}I_{2y}I_{3y}) \;-\; 0.5\,(4I_{1y}I_{2x}I_{3y}) \;-\; 0.5\,(4I_{1y}I_{2y}I_{3x}) \\
& -\, 0.5\,i\,(4I_{1y}I_{2y}I_{3y}) + 0.5\,i\,(4I_{1y}I_{2x}I_{3x}) + 0.5\,i\,(4I_{1x}I_{2y}I_{3x}) + 0.5\,i\,(4I_{1x}I_{2x}I_{3y}) \\
= {} & 2I_{1x}I_{2x}I_{3x} \;-\; 2I_{1x}I_{2y}I_{3y} \;-\; 2\, I_{1y}I_{2x}I_{3y} \;-\; 2\, I_{1y}I_{2y}I_{3x} \\
& -\, 2\,i\, I_{1y}I_{2y}I_{3y} + 2\,i\, I_{1y}I_{2x}I_{3y} + 2\,i\, I_{1x}I_{2y}I_{3x} + 2\,i\, I_{1x}I_{2x}I_{3y}
\end{aligned}
$$

Pulse sequence design challenge

Challenge 6:

Suppose in the course of a pulse sequence, you have created the state $I_{1z}I_{2z} - I_{1y}I_{2y}$. How can you transfer this state into ±2 quantum coherence by a single pulse?

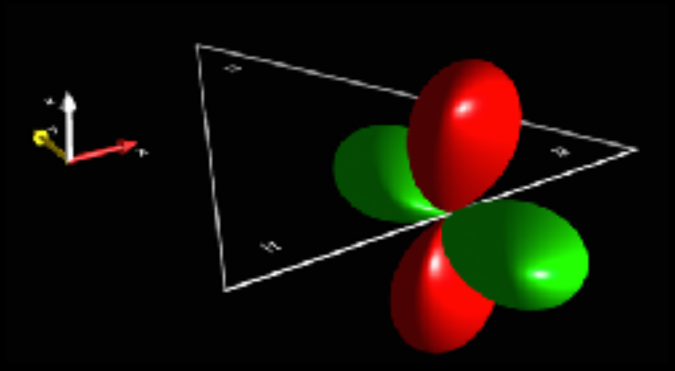
Pulse sequence design challenge

Challenge 6:

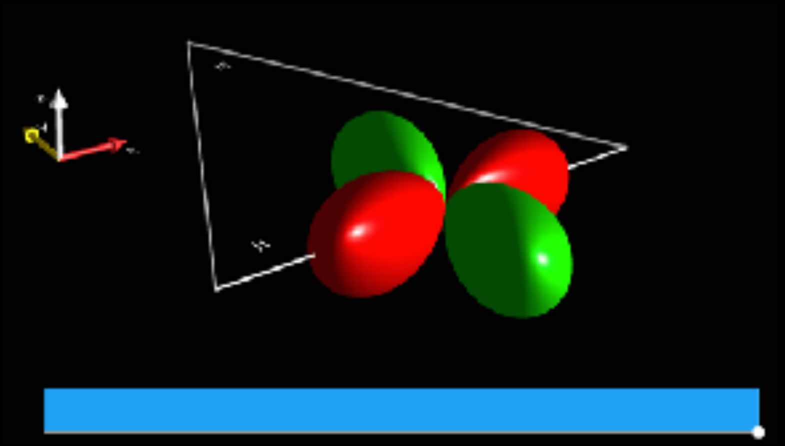
Suppose in the course of a pulse sequence, you have created the state $I_{1z}I_{2z} - I_{1y}I_{2y}$. How can you transfer this state into ±2 quantum coherence by a single pulse?

Solution:

Using the menu *Initial State > Edit Operator* create the operator $I_{1z}I_{2z} - I_{1y}I_{2y}$. The corresponding DROPS representation is indicated at the right.



The droplet representing the bilinear terms involving spins I_1 and I_2 already has the desired shape and color of ±2 quantum coherence, *except* that it is not correctly oriented! Simply rotating it by 90° around the y (or −y) axis will yield the correct orientation, i.e. a non-selective $90°_y$ (or a $90°_{-y}$) pulse yields the desired ±2 quantum coherence. This can be tested by selecting Pulse Sequence > Rotation >90° Pulse > 90°(-y) and the resulting DROPS representation at the end of the pulse is shown on the right. (Note the rectangle at the bottom, which represents the pulse, where the blue color represents the pulse phase −y.)



Define a new operator

Challenge 7:

Display the droplet corresponding to the operator $2I_{1x}I_{2x} + i\ 2I_{1z}I_{2x}$. (When the droplet is oriented properly, you will see the *SpinDrops* logo.)

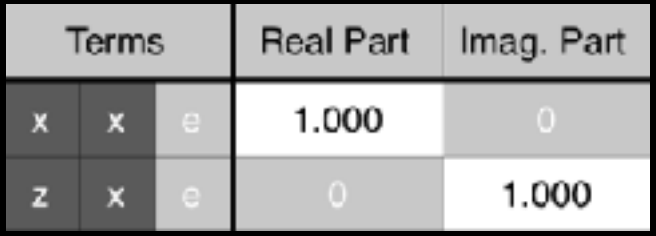
Define a new operator

Challenge 7:

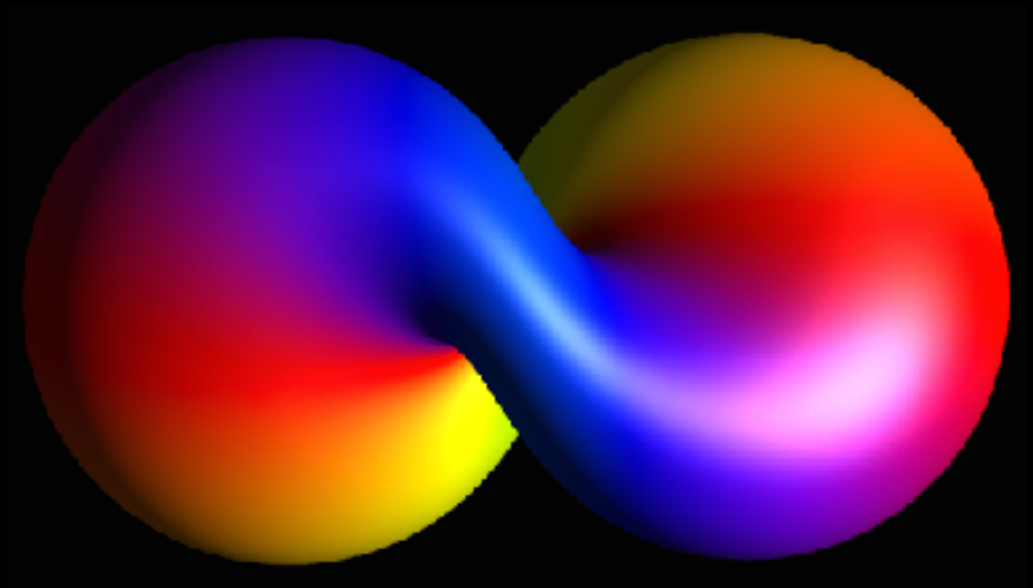
Display the droplet corresponding to the operator $2I_{1x}I_{2x} + i\ 2I_{1z}I_{2x}$. (When the droplet is oriented properly, you will see the *SpinDrops* logo.)

Solution:

Using the menu *Initial State > Edit Operator,* create the operator $2I_{1x}I_{2x} + i\ 2I_{1z}I_{1x}$. Orienting the resulting droplet in the Drops display such that the view direction is along the y axis yields the *SpinDrops* logo :-)



Terms			Real Part	Imag. Part
x	x	e	1.000	0
z	x	e	0	1.000



Rotations of operators and droplets

Challenge 8:

Starting from the term $2I_{1x}I_{2y}$, find a sequences of non-selective rotations ($90_{\pm x}$, $90_{\pm y}$, or $90_{\pm z}$) that creates all bilinear operators of the form $2I_{1a}I_{2b}$ with $a \neq b$ and $a,b \in \{x,y,z\}$.

Rotations of operators and droplets

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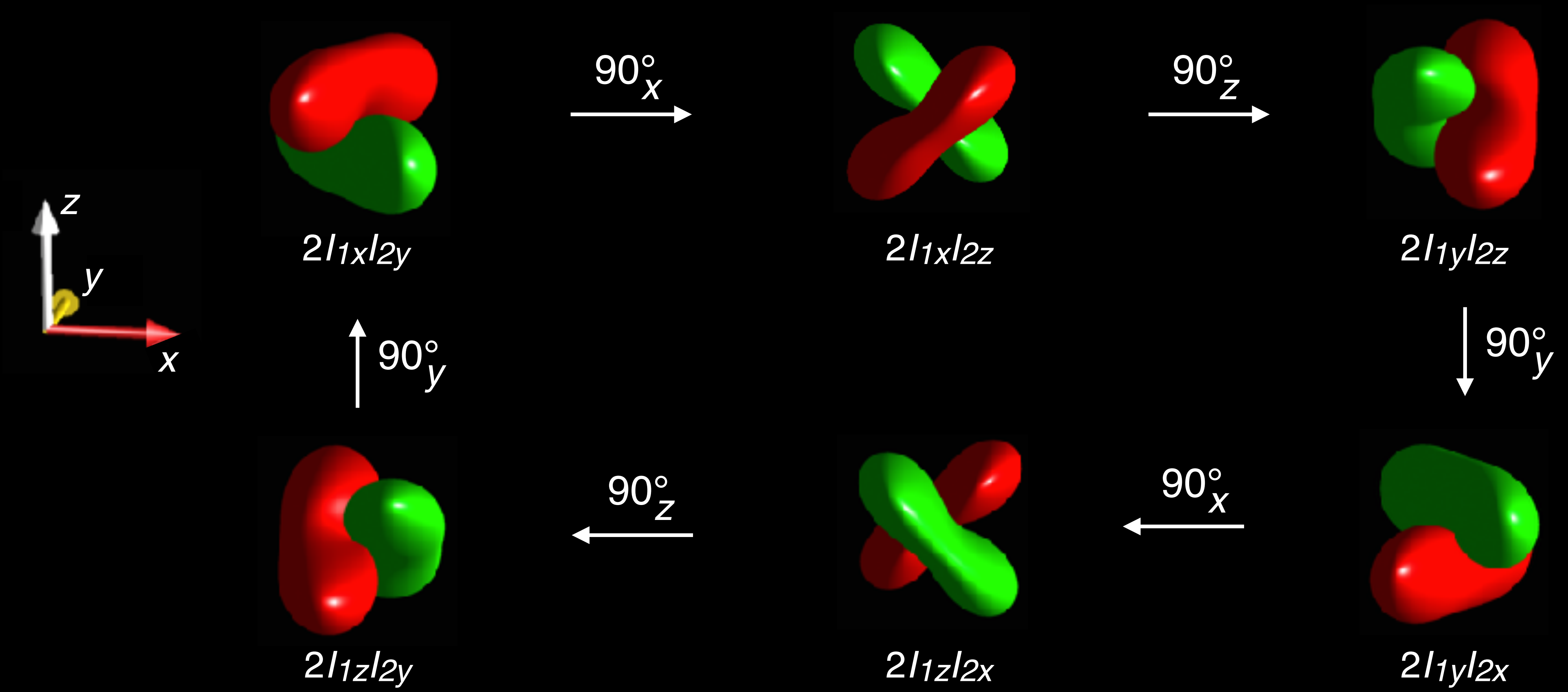
Solution:



$2I_{1x}I_{2y}$ $\xrightarrow{90^\circ_x}$ $2I_{1x}I_{2z}$ $\xrightarrow{90^\circ_z}$ $2I_{1y}I_{2z}$

$2I_{1y}I_{2z}$ $\xrightarrow{90^\circ_y}$ $2I_{1y}I_{2x}$

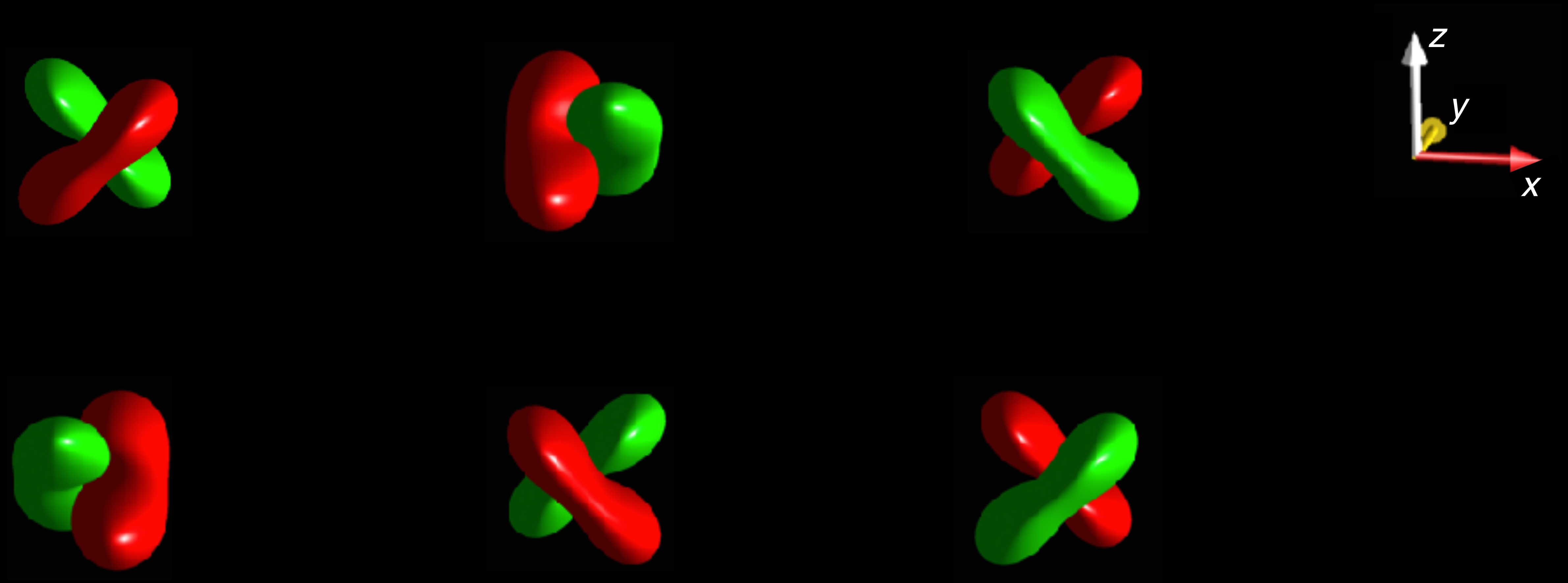
$2I_{1y}I_{2x}$ $\xrightarrow{90^\circ_x}$ $2I_{1z}I_{2x}$ $\xrightarrow{90^\circ_z}$ $2I_{1z}I_{2y}$

$2I_{1z}I_{2y}$ $\xrightarrow{90^\circ_y}$ $2I_{1x}I_{2y}$

Recognizing droplets of antiphase operators (A)

Challenge 9:

Determine for each of the following *droplets* whether it represents antiphase coherence with respect to the *first* spin ($\pm 2I_{1z}I_{2a}$ with $a \in \{x,y\}$) or with respect to the *second* spin ($\pm 2I_{1a}I_{2z}$ with $a \in \{x,y\}$)!



Recognizing droplets of antiphase operators (A)

Challenge 9:

Determine for each of the following *droplets* whether it represents antiphase coherence with respect to the *first* spin ($\pm 2I_{1z}I_{2a}$ with $a \in \{x,y\}$) or with respect to the *second* spin ($\pm 2I_{1a}I_{2z}$ with $a \in \{x,y\}$)!

Solution:

This challenge can be solved by simply observing the "kissing beans' head tilt" (c.f. Help > DROPS).

"right tilt"

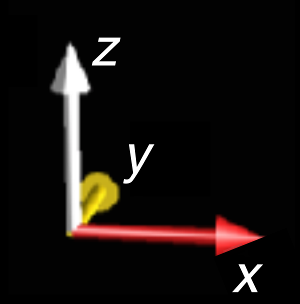
$\pm 2I_{1a}I_{2z}$

"left tilt"

$\pm 2I_{1z}I_{2a}$

"left tilt"

$\pm 2I_{1z}I_{2a}$



"right tilt"

$\pm 2I_{1a}I_{2z}$

"left tilt"

$\pm 2I_{1z}I_{2a}$

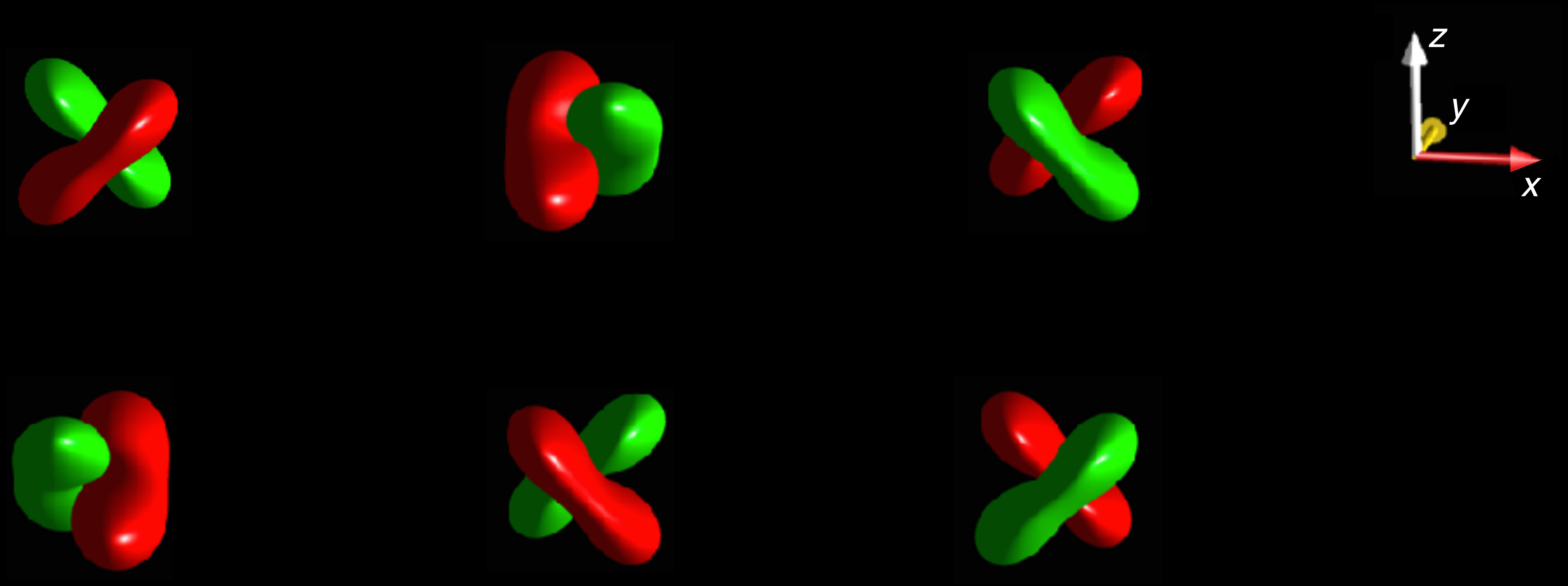
"right tilt"

$\pm 2I_{1a}I_{2z}$

Recognizing droplets of antiphase operators (B)

Challenge 10:

Determine for each of the *droplets* the *exact* form of the corresponding antiphase operator!



Recognizing droplets of antiphase operators (B)

Challenge 10:

Determine for each of the *droplets* the *exact* form of the corresponding antiphase operator!

Solution:

Since (based on the “kissing beans’ head tilt”) it is clear which of the two single-spin operators is I_z, it remains to determine whether the remaining single spin operator is I_x, I_y, I_{-x}, or I_{-y}. The exact form of the operator can be found using the right-hand rule explained in *Help > DROPS*.

“right tilt”

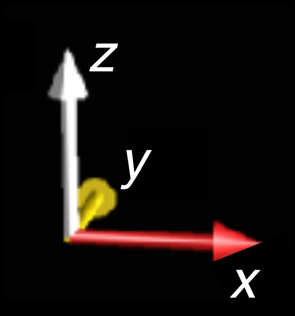
$2I_{1x}I_{2z}$

“left tilt”

$2I_{1z}I_{2y}$

“left tilt”

$2I_{1z}I_{2x}$



“right tilt”

$2I_{1y}I_{2z}$

“left tilt”

$-2I_{1z}I_{2x}$

“right tilt”

$-2I_{1x}I_{2z}$

Symmetry of antiphase operators under 180° rotations (A)

Challenge 11: Verify that the following symmetry relations of anti-phase operators under 180° rotations are faithfully represented by the corresponding antiphase droplets!

(a) $2I_{1x}I_{2z} \xrightarrow{180^\circ_x} -2I_{1x}I_{2z}$ (b) $2I_{1x}I_{2z} \xrightarrow{180^\circ_y} 2I_{1x}I_{2z}$ (c) $2I_{1x}I_{2z} \xrightarrow{180^\circ_z} -2I_{1x}I_{2z}$

(d) $2I_{1y}I_{2z} \xrightarrow{180^\circ_x} 2I_{1y}I_{2z}$ (e) $2I_{1y}I_{2z} \xrightarrow{180^\circ_y} -2I_{1y}I_{2z}$ (f) $2I_{1y}I_{2z} \xrightarrow{180^\circ_z} -2I_{1y}I_{2z}$

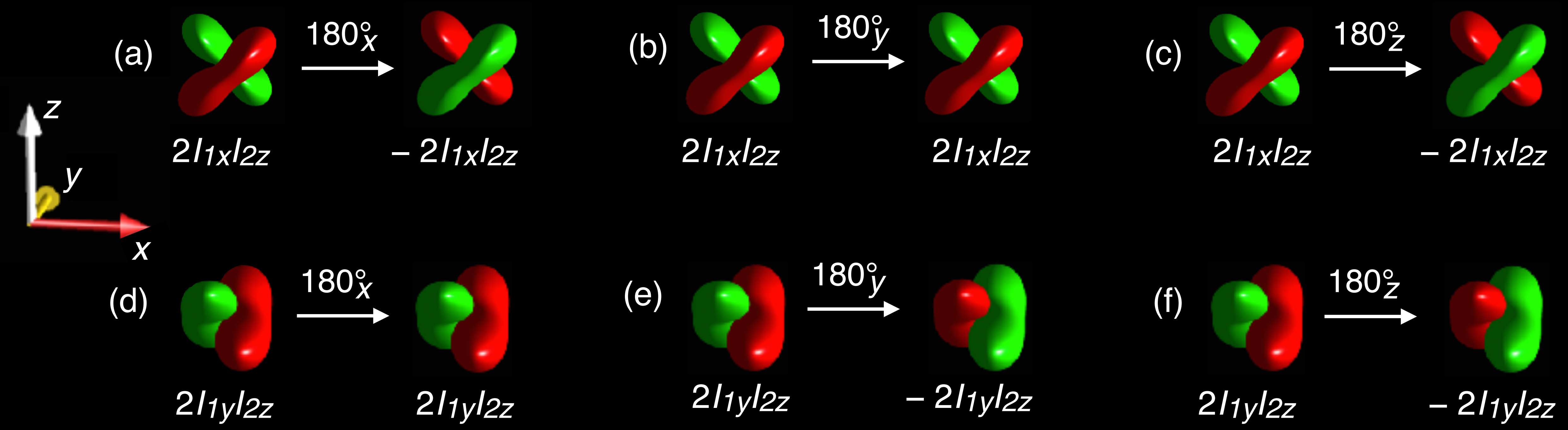
Symmetry of antiphase operators under 180° rotations (A)

Challenge 11: Verify that the following symmetry relations of anti-phase operators under 180° rotations are faithfully represented by the corresponding antiphase droplets!

(a) $2I_{1x}I_{2z} \xrightarrow{180^\circ_x} -2I_{1x}I_{2z}$ (b) $2I_{1x}I_{2z} \xrightarrow{180^\circ_y} 2I_{1x}I_{2z}$ (c) $2I_{1x}I_{2z} \xrightarrow{180^\circ_z} -2I_{1x}I_{2z}$

(d) $2I_{1y}I_{2z} \xrightarrow{180^\circ_x} 2I_{1y}I_{2z}$ (e) $2I_{1y}I_{2z} \xrightarrow{180^\circ_y} -2I_{1y}I_{2z}$ (f) $2I_{1y}I_{2z} \xrightarrow{180^\circ_z} -2I_{1y}I_{2z}$

Solution: Applying the 180° pulses to the antiphase droplets yields the expected results. For example, a 180°_y pulse reproduces the shape and colors of the $2I_{1x}I_{2z}$ droplet (case b), whereas a 180°_x pulse inverts the colors (and hence the sign) of the $2I_{1x}I_{2z}$ droplet (case a).



Comparing the speed of coherence transfer

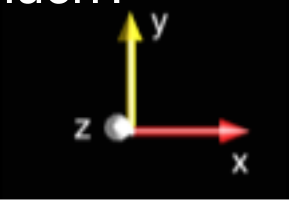
Challenge 12:

Compare the time required to transfer the initial state I_{1x} to I_{2x} in a homonuclear two-spin system when using either a sequence of delays and pulses or an isotropic mixing (TOCSY) sequence for a given coupling constant J_{12}. Which sequence is faster and by how much?

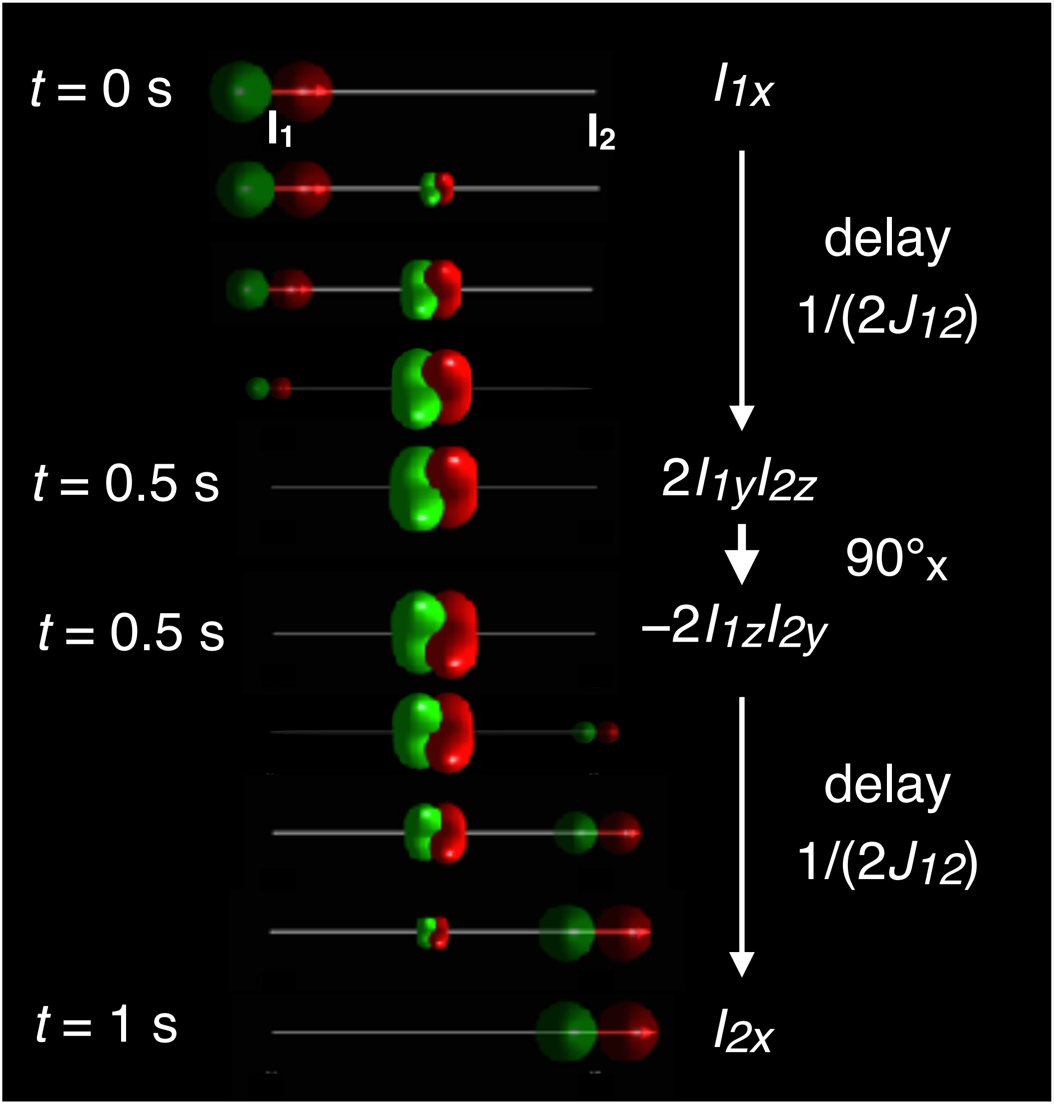
Comparing the speed of coherence transfer

Challenge 12:

Compare the time required to transfer the initial state I_{1x} to I_{2x} in a homonuclear two-spin system when using either a sequence of delays and pulses or an isotropic mixing (TOCSY) sequence for a given coupling constant J_{12}. Which sequence is faster and by how much?



Solution:



$t = 0$ s I_{1x}

I_1 I_2

delay $1/(2J_{12})$

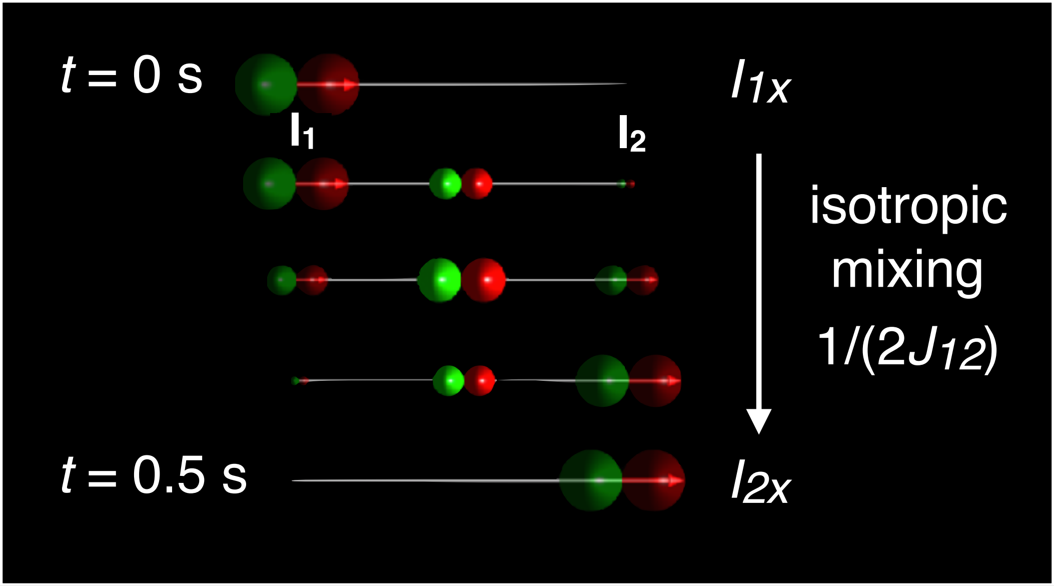
$t = 0.5$ s $2I_{1y}I_{2z}$

$90°_x$

$t = 0.5$ s $-2I_{1z}I_{2y}$

delay $1/(2J_{12})$

$t = 1$ s I_{2x}



$t = 0$ s I_{1x}

I_1 I_2

isotropic mixing $1/(2J_{12})$

$t = 0.5$ s I_{2x}

For $J_{12} = 1$ Hz (and $\nu 1 = \nu 2 = 0$ Hz), simulations are shown for the sequence $1/(2J_{12})$ - $90°_x$ - $1/(2J_{12})$ (left) and for isotropic mixing (top). The isotropic mixing sequence only requires half the amount of time compared to the INEPT-type transfer, i.e. it is twice as fast.

Seeing coherence orders

Challenge 13:

Which coherence orders *p* are contained in the following operators?

(a) $2I_{1x}I_{2z}$ (b) $2I_{1x}I_{2x}$ (c) $I_{1x}I_{2x} - I_{1y}I_{2y}$ (d) $I_{1x}I_{2x} + I_{1y}I_{2y}$

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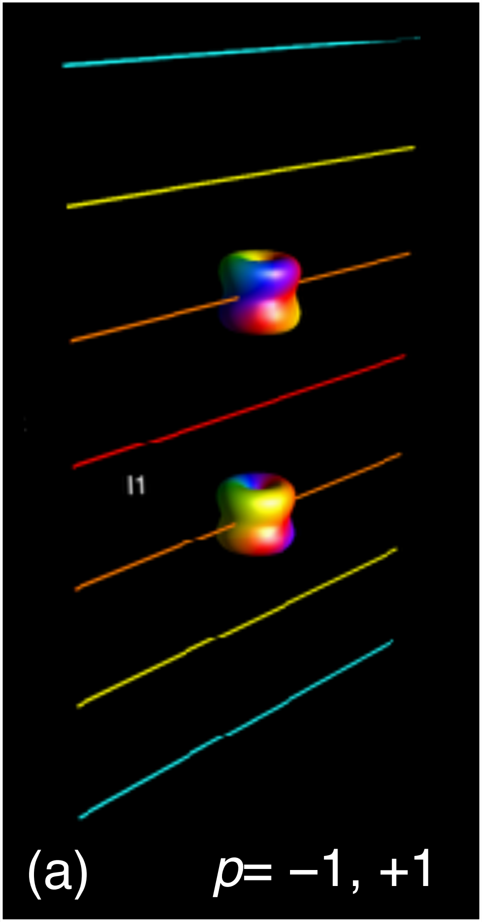
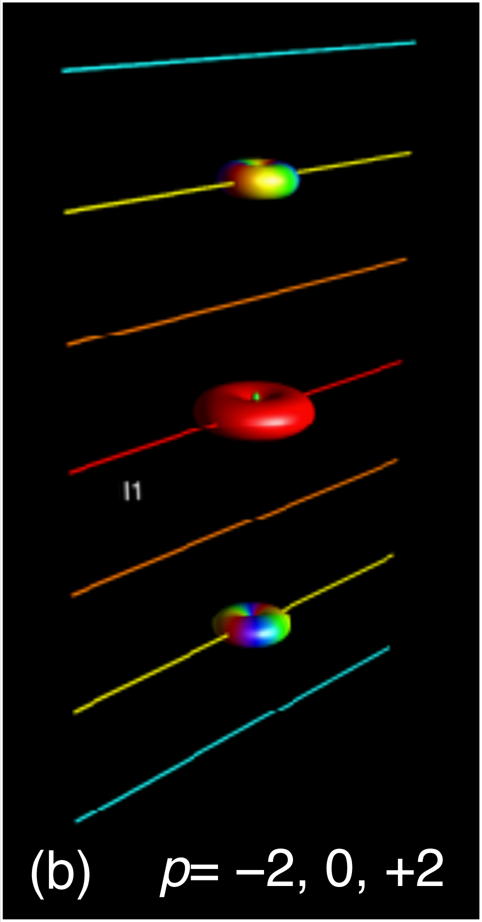
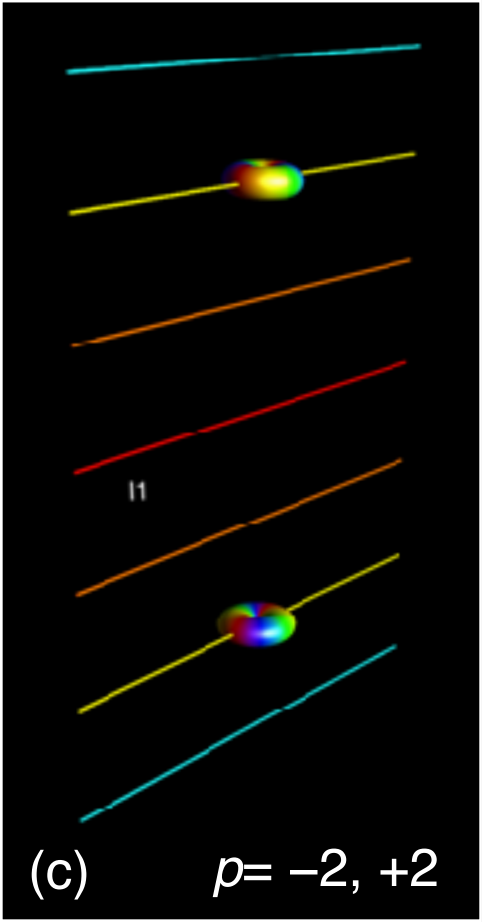
Solution: Create the terms using the *Initial State > Edit Operator* menu. Choose *Display Options > Separation > Coh. Order p* to see the corresponding droplet terms separated based on coherence order:



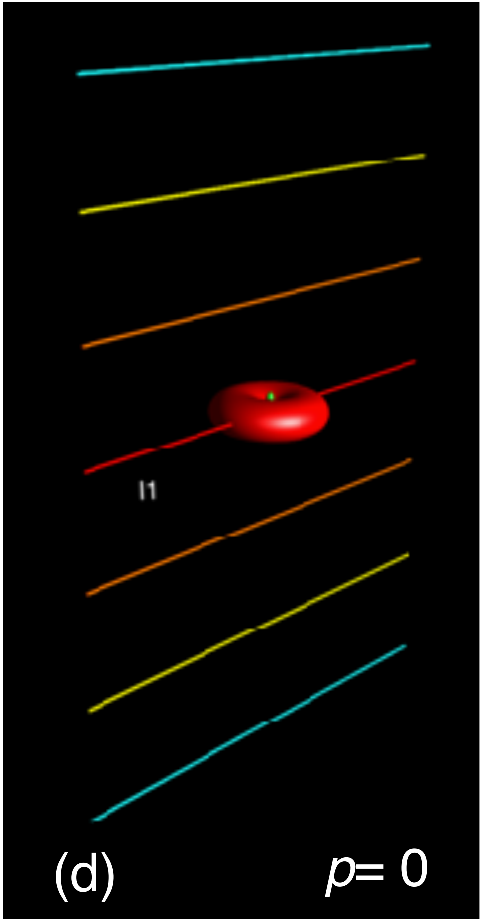
(a) $p = -1, +1$



(b) $p = -2, 0, +2$



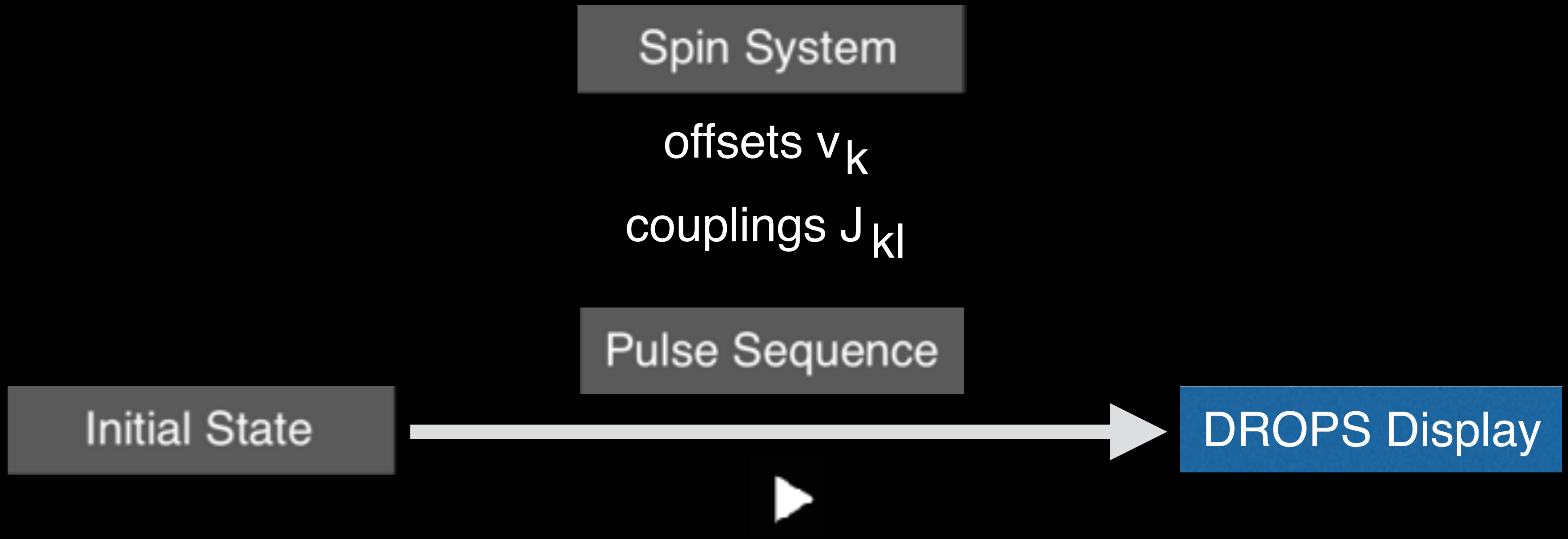
(c) $p = -2, +2$



(d) $p = 0$

FAQ

What do I need to do to see the effect of a pulse sequence?



Spin System

offsets ν_k

couplings J_{kl}

Pulse Sequence

Initial State

DROPS Display

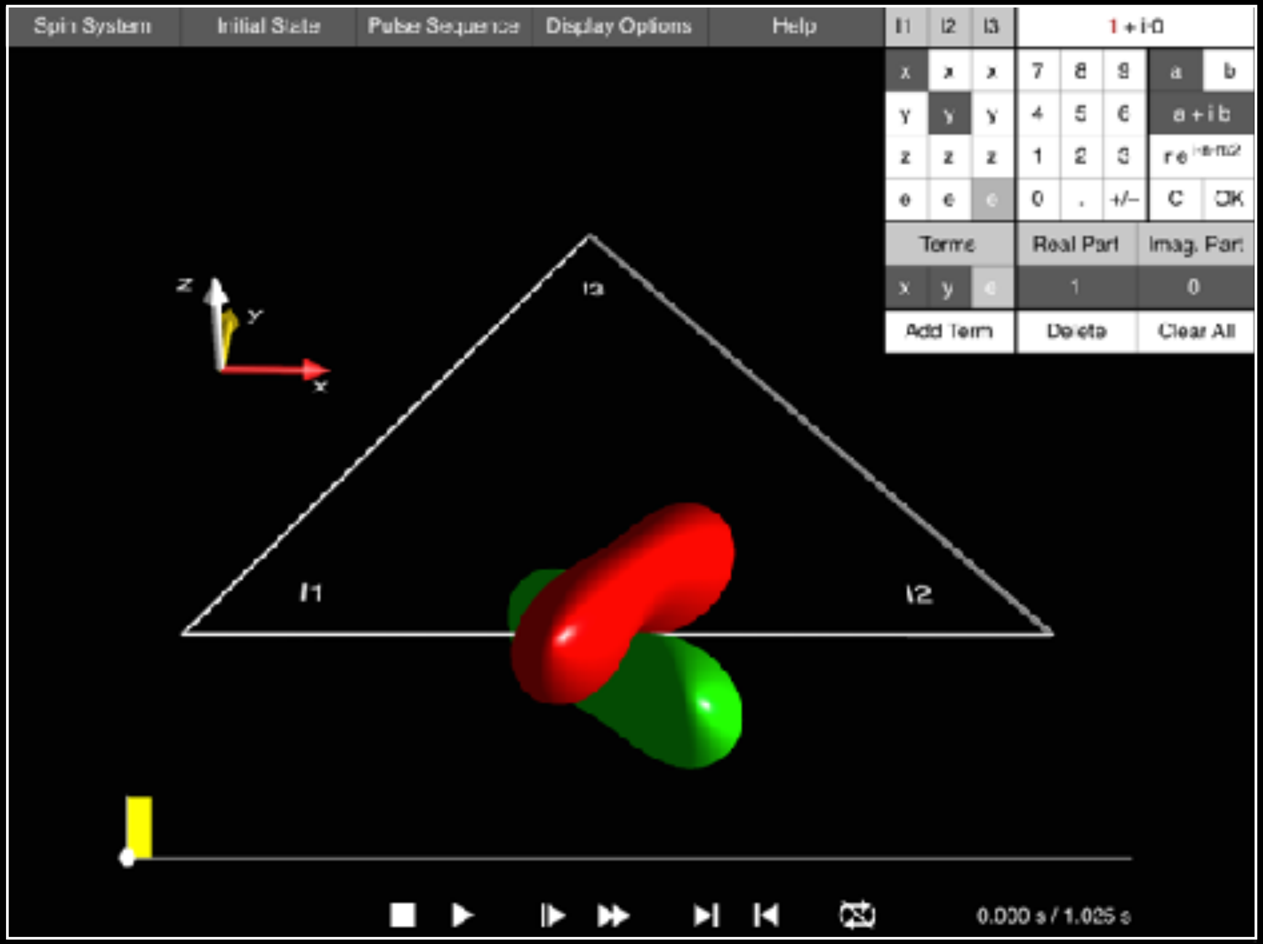
The simulation requires the definition of the spin system and its parameters (offset frequencies and coupling constants). Also make sure the desired initial state and the pulse sequence are specified. Now the simulation can be started with the play button and the DROPS display shows the effect on the state of the spin system in real time.

How can I see what a particular operator looks like?

Simply define the operator of interest in the menu *Initial State > Define Operator*

In this example, the operator $2I_{1x}I_{2y}$ is displayed.

(In the menu *Edit Operator*, it is defined using the short-hand notation “xye”.)



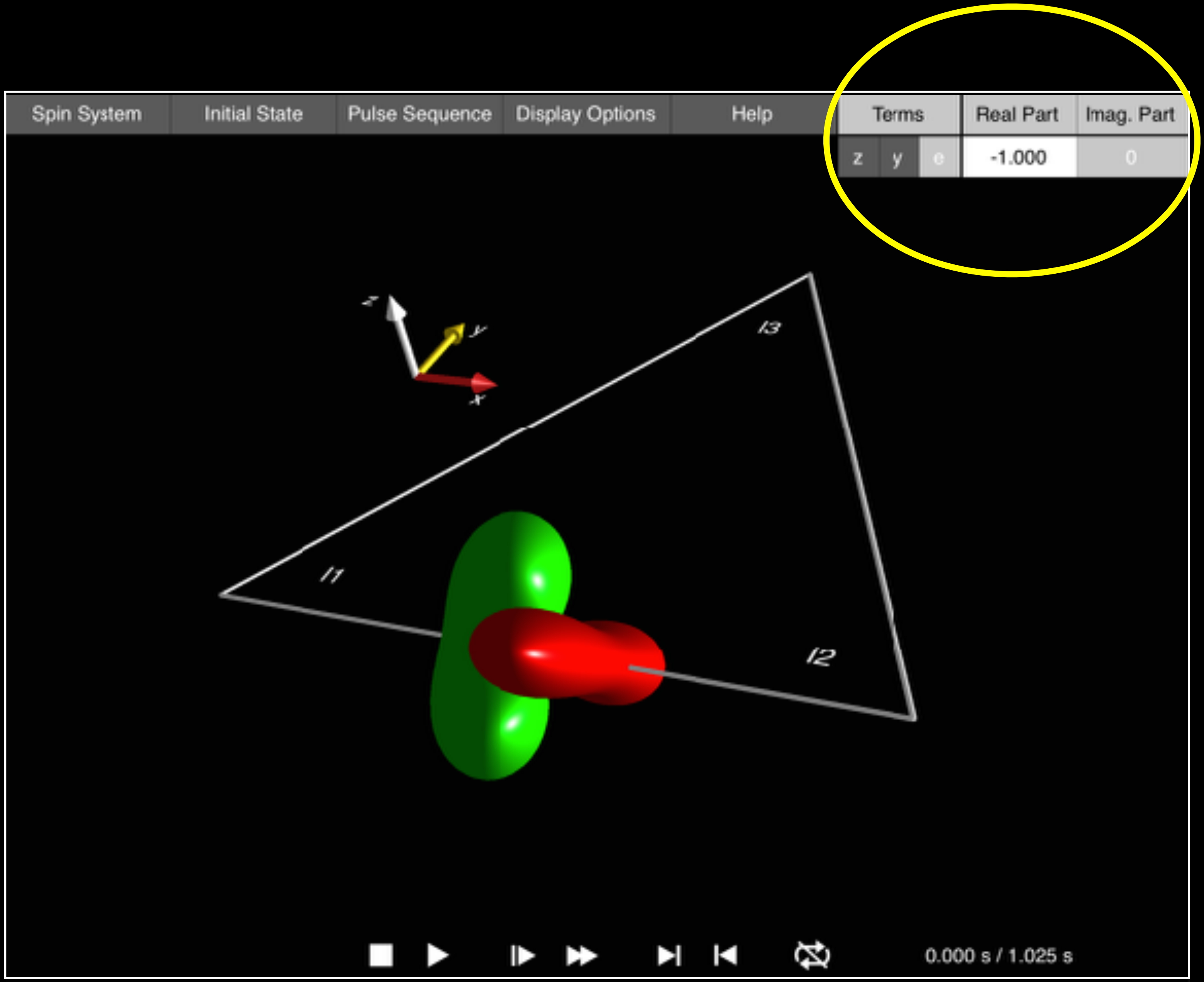
Tip 1: Before defining the operator, make sure the time slider is at the beginning of the selected pulse sequence. (In order to actually see the defined operator and not what it has evolved to during the pulse sequence.) A simple way to do this is to press the ■ button.

Tip 2: To have more space on the screen, you can choose *Display Options > Hide Seq. Plot.*

Tip 3: The triangle can be removed by setting all couplings to 0 Hz (go to *Spin System > Parameters*). To hide the parameter sliders, select Spin Systems > Hide Parameters.

How can I see which product operators are represented by a given DROPS display?

To see the current list of product operators (yellow ellipse), select *Display Options > List Prod. Ops.*



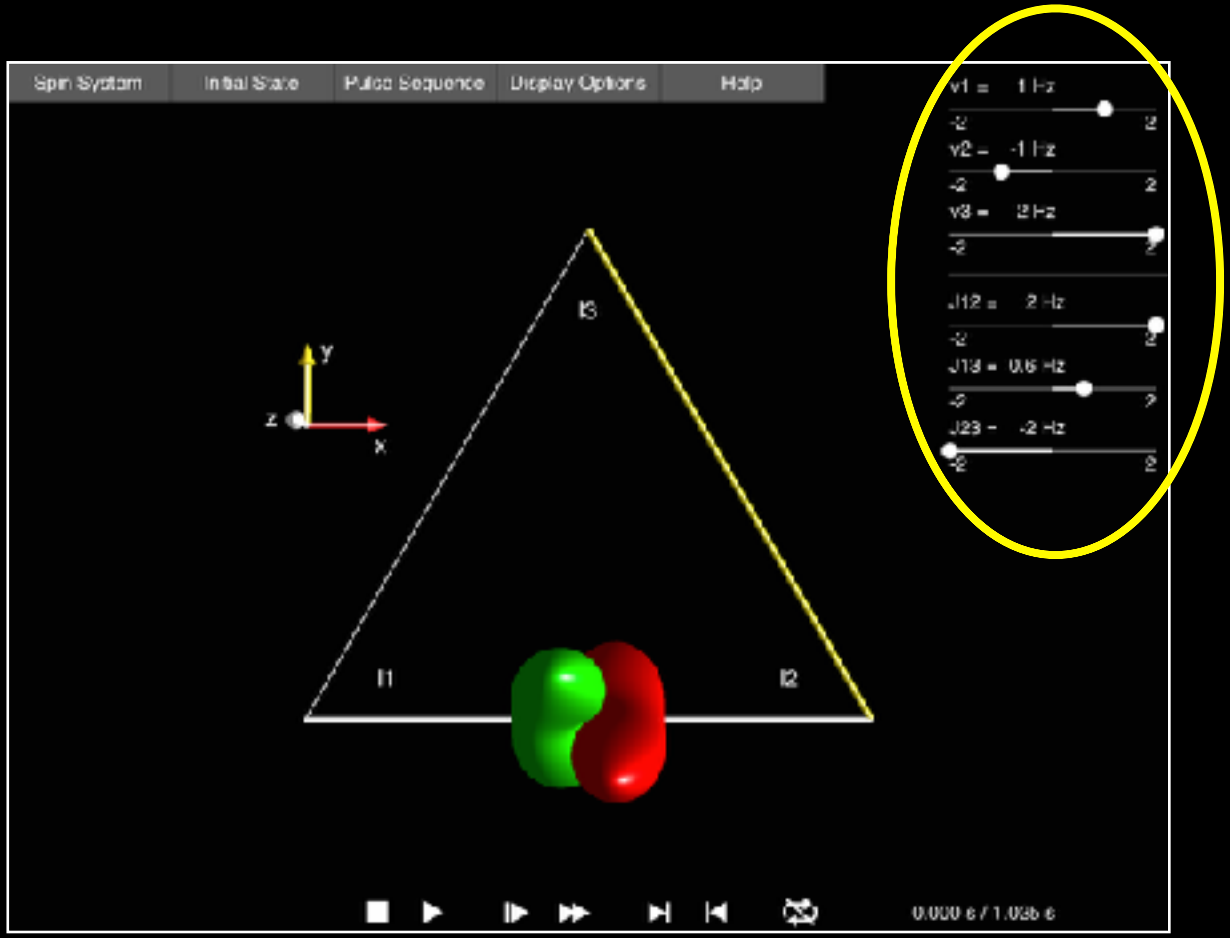
Terms	Real Part	Imag. Part
z y e	-1.000	0

The Cartesian product operator terms are displayed using the three-letter shorthand notation (see *Help > Tutorial*).

In this example, the DROPS display shows “–1 zye”, which is the shorthand notation for the Cartesian product operator $-2I_{1z}I_{2y}$.

How can I see (and modify) the current frequency offsets and coupling constants of the spins system?

Select *Spin System > Parameters*



v1 = 1 Hz
-2 2
v2 = -1 Hz
-2 2
v3 = 2 Hz
-2 2
J12 = 2 Hz
-2 2
J13 = 0.6 Hz
-2 2
J23 = -2 Hz
-2 2

The parameter sliders and the current values of the parameters are displayed at the top right corner of the screen (yellow ellipse).

In this example, the offset frequencies of the first, the second, and the third spin are 1 Hz, -1 Hz, and 2 Hz, respectively.

The coupling constants are
J12 = 2 Hz, J13 = 0.6 Hz, and J23 = -2 Hz.

Tip 1: The relative size and sign of the coupling constants is represented by the thickness and color (positive: white; negative: yellow) of the lines connecting the corresponding spins.

Tip 2: You can choose discrete or smooth slider steps in *Display Options > Slider Steps.*

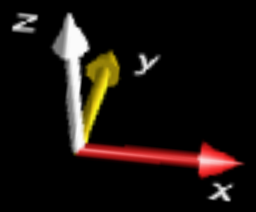
Tip 3: You can hide the parameter sliders selecting *Spin System > Hide Parameters.*

How do I choose the initial state of the spin system?

In the menu *Initial State*, a selection of initial states of interest is presented. In a typical experiments, you may be interested to start e.g. with z magnetization of the first spin of of all spins. Examples of operator you can select are given on the following pages.

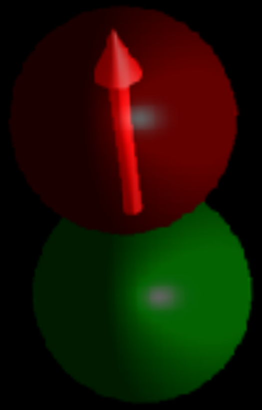
I1z	*z* magnetization of the first spin
I1x	*x* magnetization of the first spin
I1(+)	+1-quantum coherence of the first spin
I1z+I2z+I3z	*z* magnetization of the first, the second, and the third spin
MQ (x/y ops.)	Multiple-quantum operators with quantum order (+p) AND (-p) based on real combination of Cartesian product operators
MQ (+/- ops.)	Multiple-quantum operators with quantum order (+p) OR (-p) based on raising and lowering operators
Singlet(12)	The traceless part of the singlet state involving the first and second spin
Edit Operator	This option makes it possible to edit the chosen initial density operator and hence to generate any desired operator of interest

Examples of States and Droplets of a Single Spin



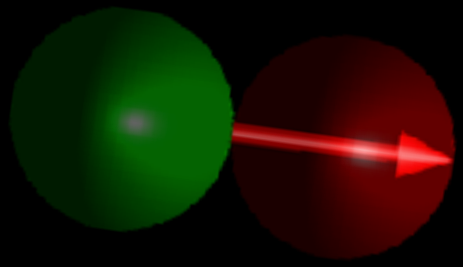
I1z

“z magnetization” I_{1z}



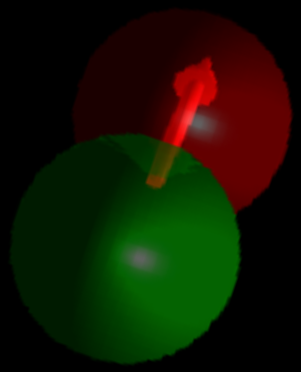
I1x

“x magnetization” I_{1x}



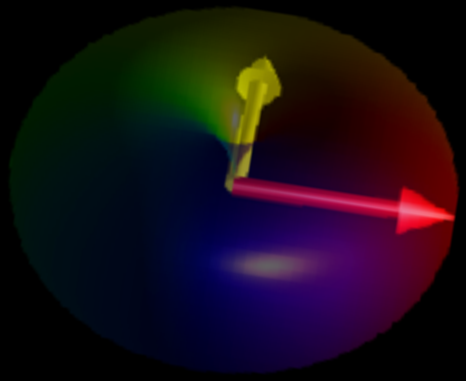
I1y

“y magnetization” I_{1y}



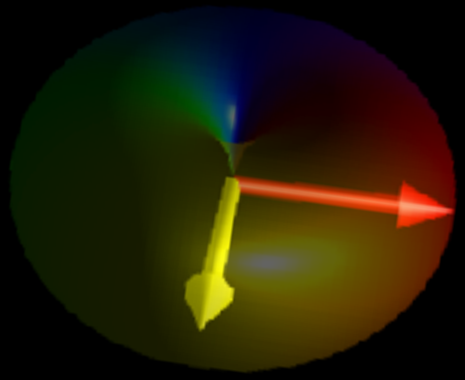
I1(+)

+1-quantum coherence $I_{1x} + \mathrm{i}\, I_{1y}$



I1(-)

–1-quantum coherence $I_{1x} - \mathrm{i}\, I_{1y}$

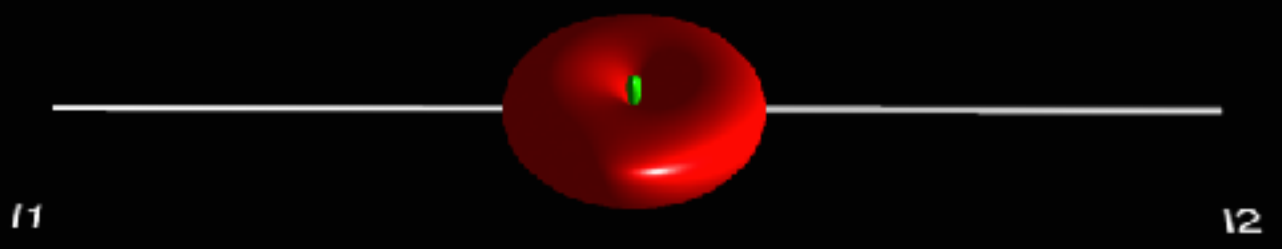


Examples of Zero-Quantum Coherences Involving Two Spins

0Qx(I1,I2)

zero-quantum *x* coherence

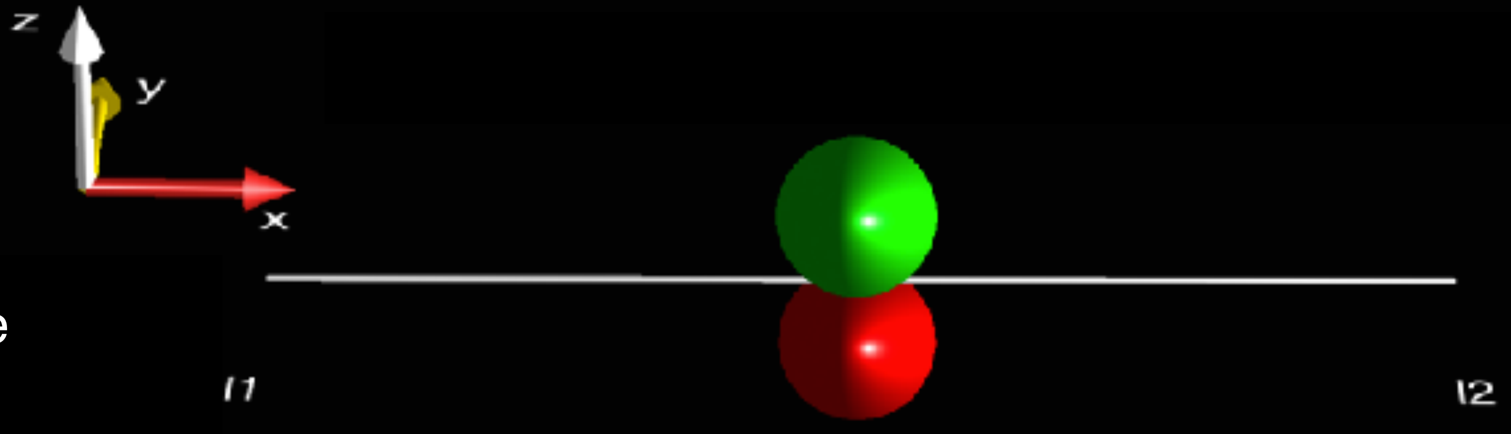
$I_{1x}I_{2x} + I_{1y}I_{2y}$



0Qy(I1,I2)

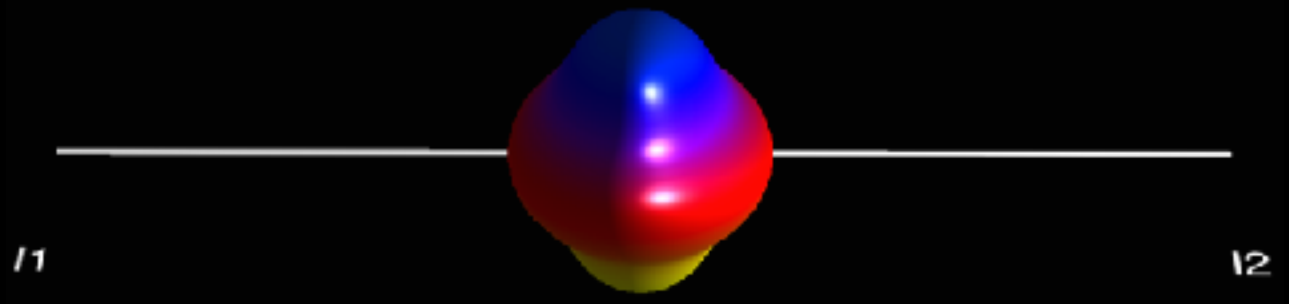
zero-quantum *y* coherence

$I_{1y}I_{2x} - I_{1x}I_{2y}$



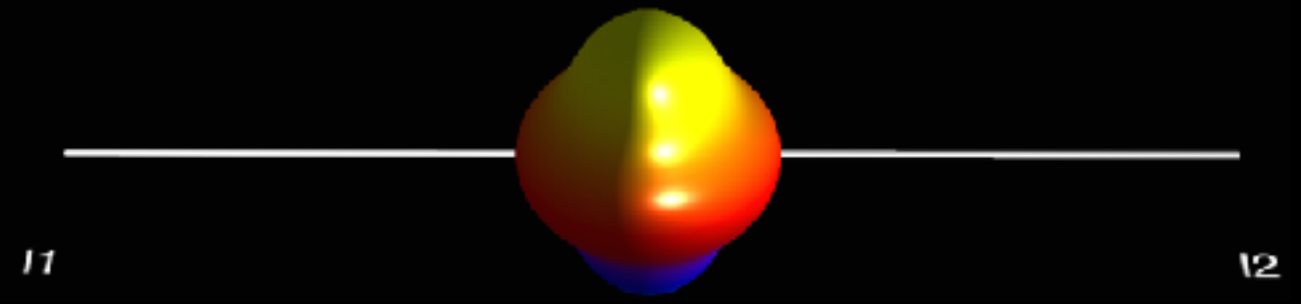
I1(+)*I2(-)

$I_1^+ I_2^-$



I1(-)*I2(+)

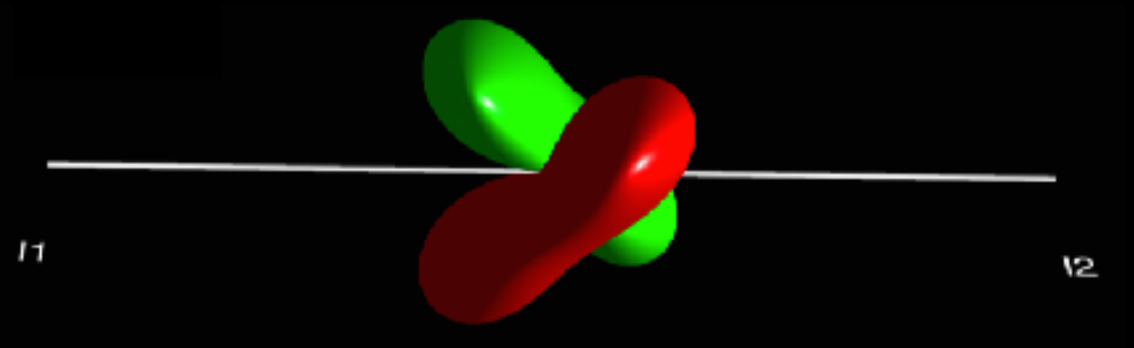
$I_1^- I_2^+$

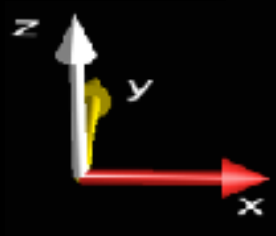


Examples of Single-Quantum Coherences Involving Two Spins

2*I1x*I2z

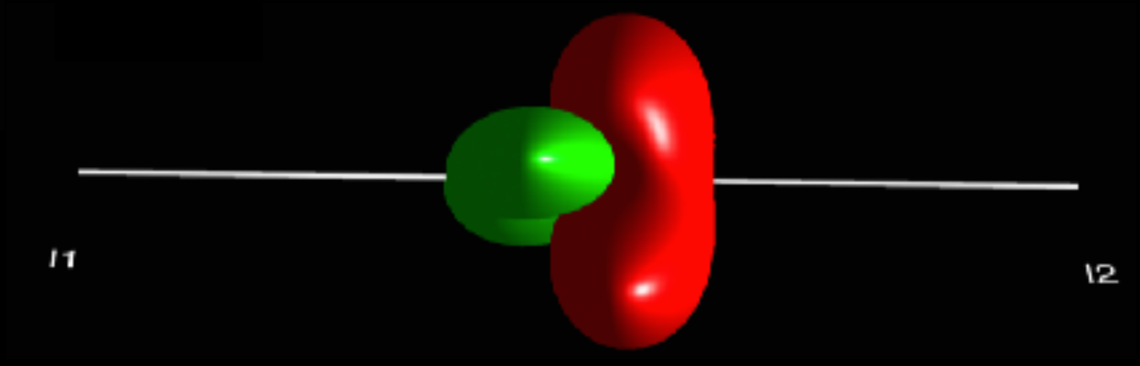
antiphase *x* coherence $2I_{1x}I_{2z}$





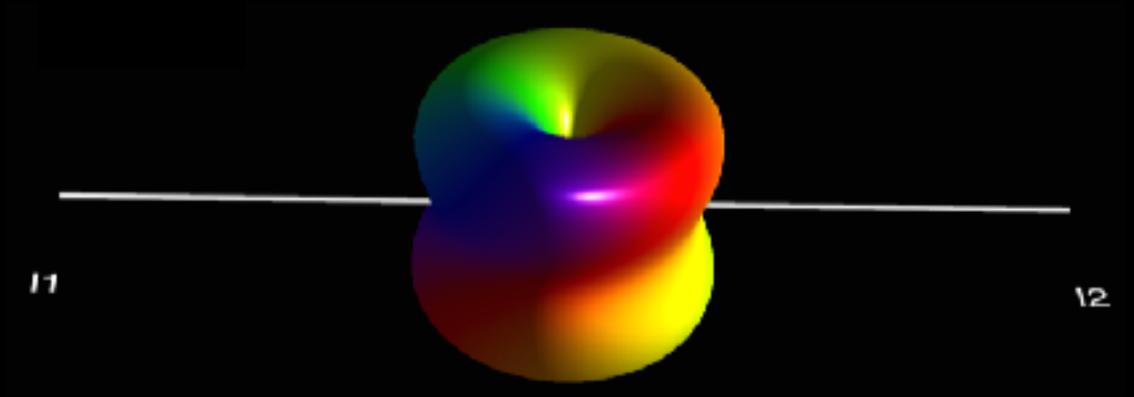
2*I1y*I2z

antiphase *y* coherence $2I_{1y}I_{2z}$



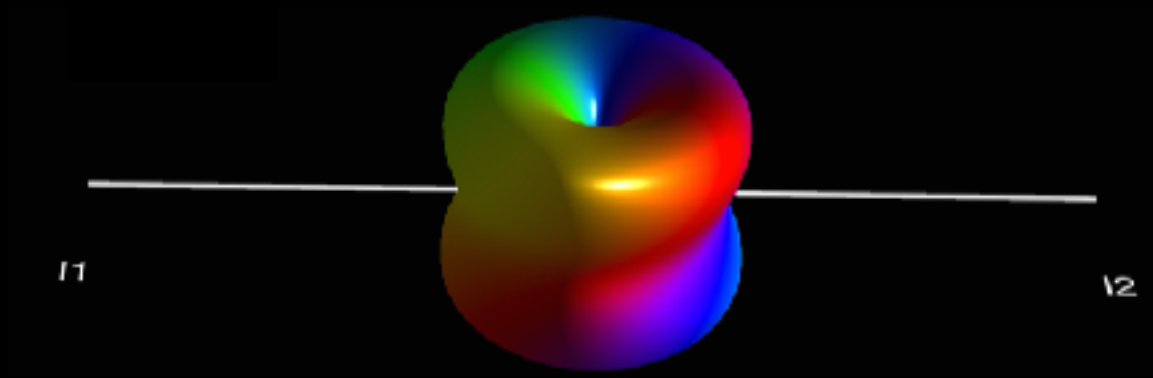
2*I1(+)*I2z

+1 quantum antiphase coherence $2I_1^+I_{2z}$



2*I1(-)*I2z

−1 quantum antiphase coherence $2I_1^-I_{2z}$

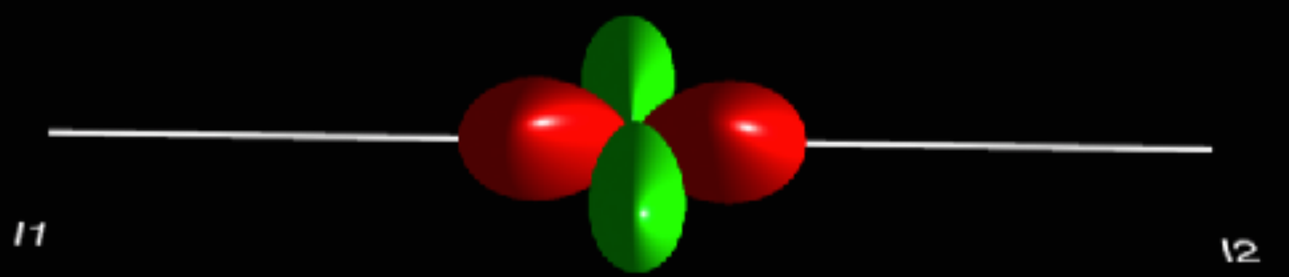


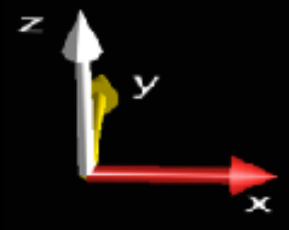
Examples of Double-Quantum Coherences Involving Two Spins

2Qx(I1,I2)

double-quantum *x* coherence

$I_{1x}I_{2x} - I_{1y}I_{2y}$

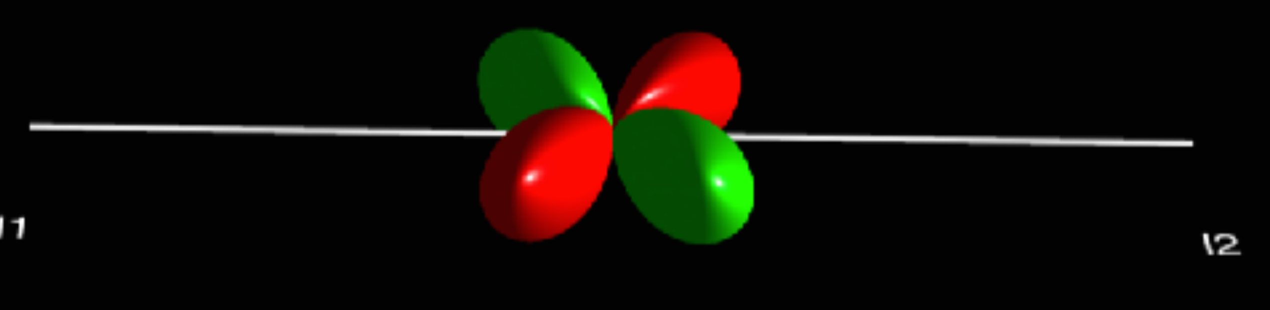




2Qy(I1,I2)

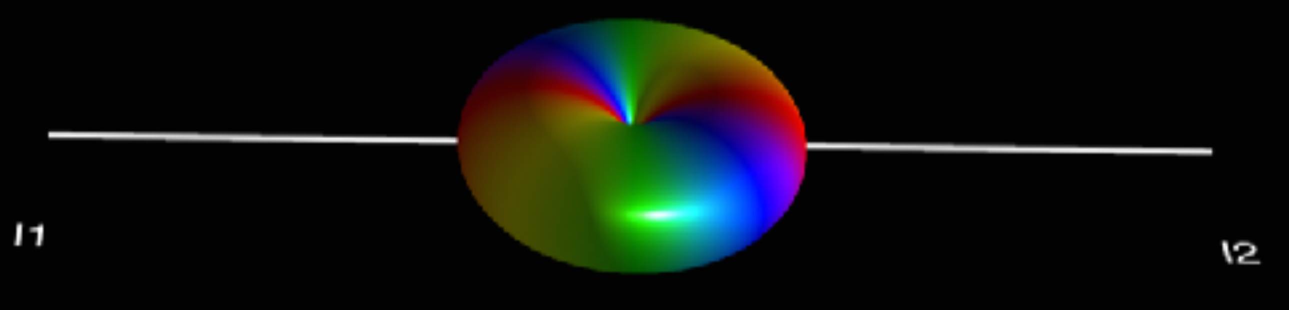
double-quantum *y* coherence

$I_{1y}I_{2x} + I_{1x}I_{2y}$



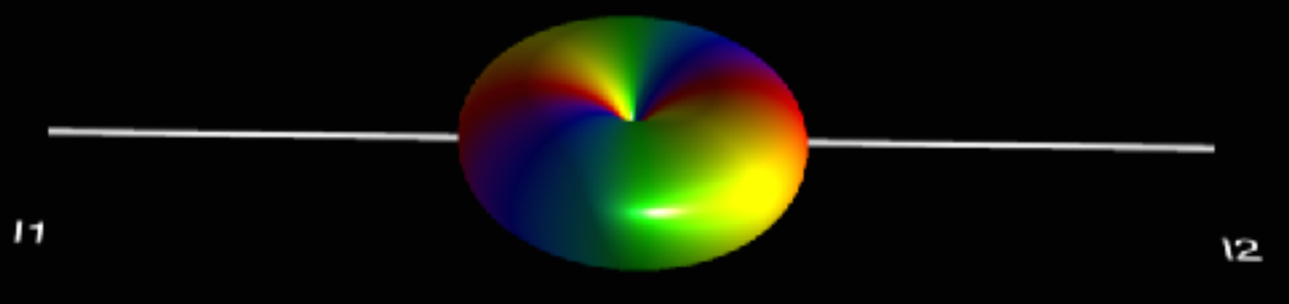
I1(+)*I2(+)

(+2)-quantum coherence $I_1^{+} I_2^{+}$



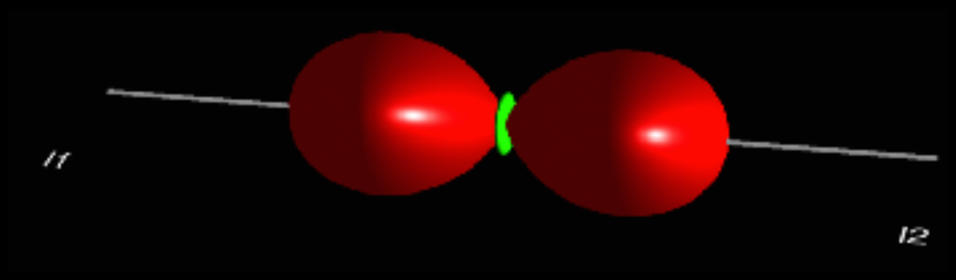
I1(-)*I2(-)

(–2)-quantum coherence $I_1^{-} I_2^{-}$



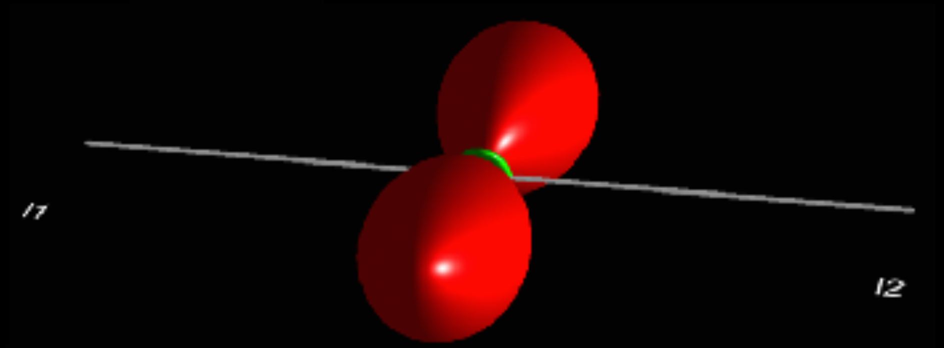
Additional Examples of Bilinear Operators Involving Two Spins

$2I_{1x}I_{2x}$



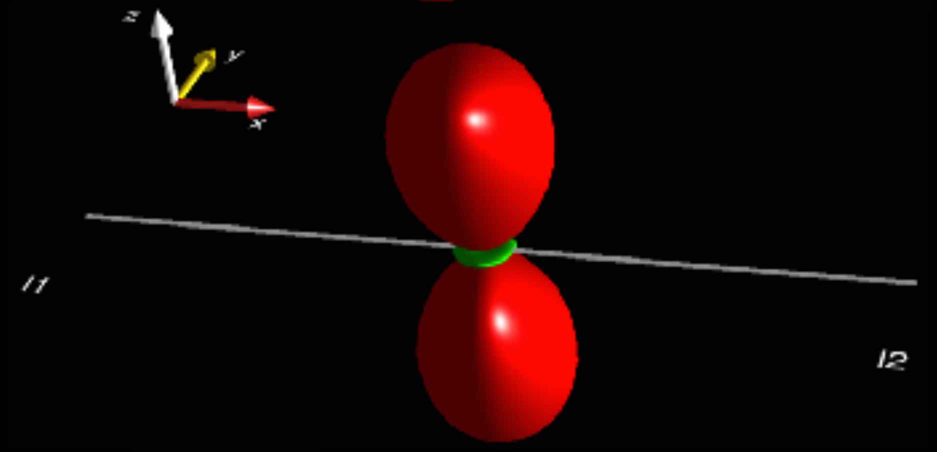
1	xx

$2I_{1y}I_{2y}$



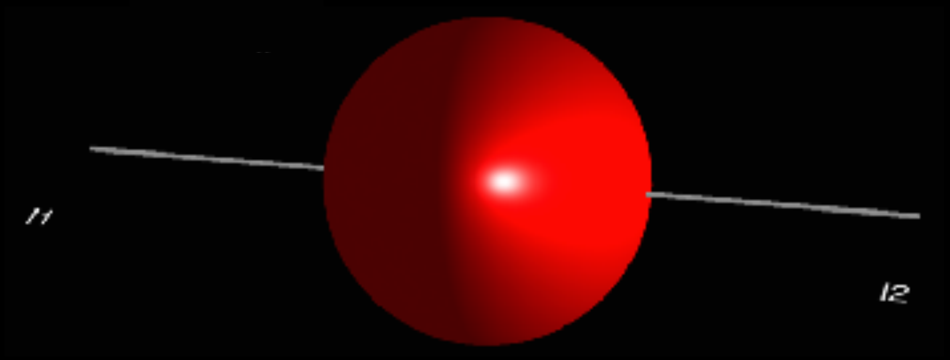
1	yy

$2I_{1z}I_{2z}$



1	zz

$2I_{1x}I_{2x} + 2I_{1y}I_{2y} + 2I_{1z}I_{2z}$



1	xx
1	yy
1	zz

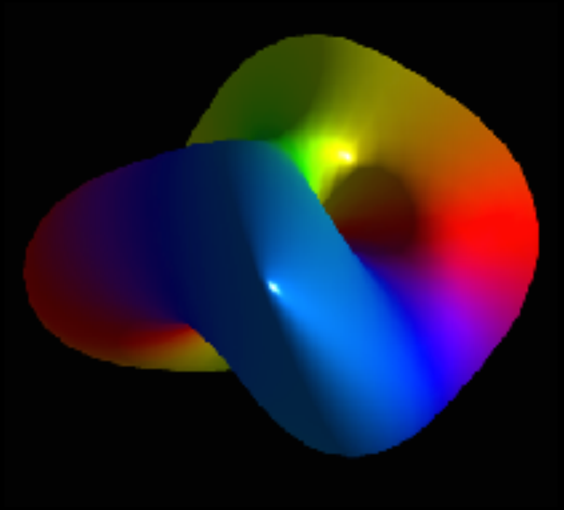
How Can I Take a Screenshot of my DROPS Display?

A screen shot of the iPad or iPhone can be made by simultaneous clicking the home and power buttons.

The screenshot will be saved in the Camera Roll. To see the screen shot, use the standard "Photos" app on the home screen.

Mathematical Background

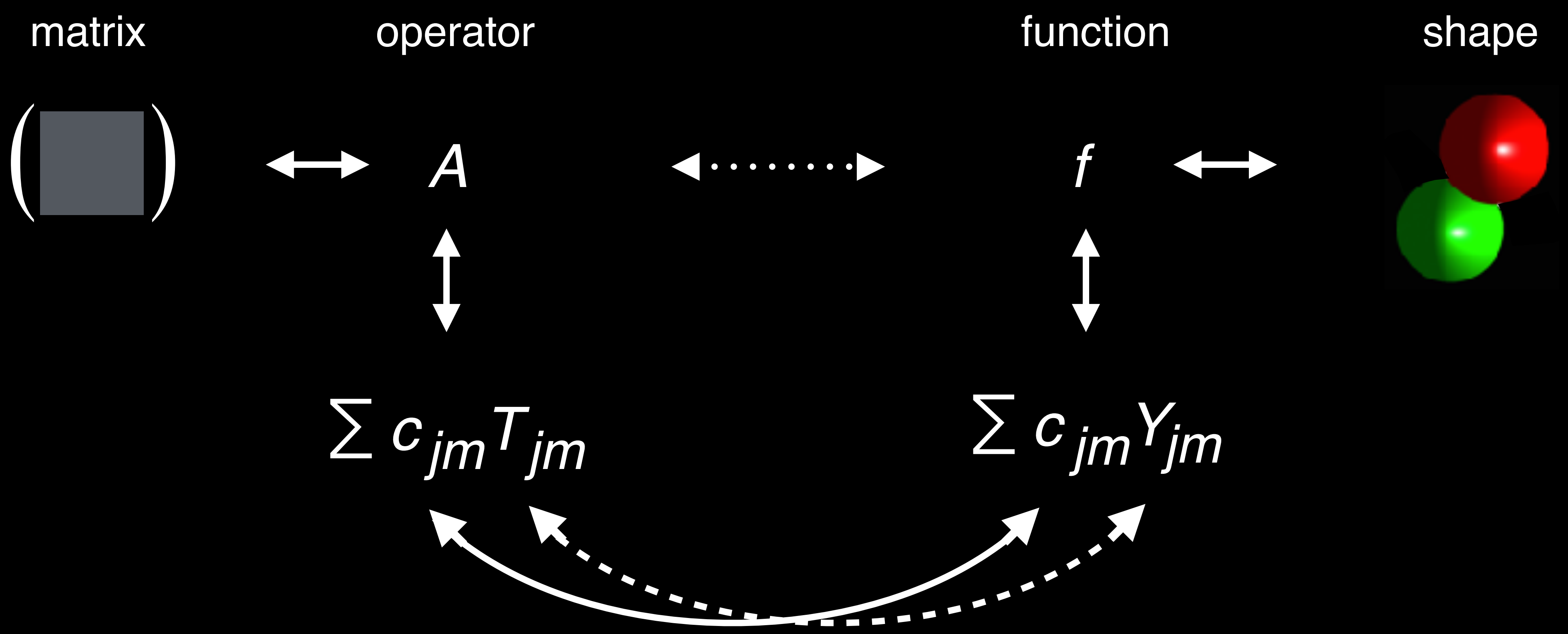
Mathematical Background of the DROPS Visualization



In order to use the DROPS representation to visualize e.g. the state of a coupled spin system, it is *not* necessary to understand the mathematical details of the mapping between quantum-mechanical operators and their DROPS representation. (Similarly, in order to use the well-known vector picture to visualize the state of uncoupled spins, it is not necessary to understand the mathematical details of the mapping between quantum-mechanical operators for two-level systems and their vector representation via the expectation values of the spin operators I_x, I_y, and I_z etc.).

Still, in may be interesting to learn more about the mathematical background of this mapping and the connection to Wigner representations. In the following, we summarize some of the underlying ideas. For more details, we refer to the manuscript "*Visualizing states and operators of coupled spins systems*“ by A. *Garon et al (2015)* and to A. Garon's thesis „*On a new visualization tool for quantum systems and on a time-optimal control problem for quantum gates*“ (see *Help > References*).

Wigner Functions of Single Spins



matrix

operator

function

shape

A

f

$\sum c_{jm} T_{jm}$

$\sum c_{jm} Y_{jm}$

For a system consisting only of a single spin (not necessarily spins 1/2), it is always possible to express an operator (such as the density operator encoding the state of the spin) as a linear combination of tensor operators T_{jm} with (in general complex) coefficients c_{jm}. By using the natural mapping between tensor operators T_{jm} and spherical harmonics Y_{jm}, is it possible to represent any operator A by a function f on a sphere, which can have complex values and which can be plotted as a three-dimensional shape: for a given point s of the unit sphere, the complex number $f(s)$ can be written as $r(s)\, e^{i\phi(s)}$ and it can be represented by a point with distance $r(s)$ from the origin and a color to represent the phase $\phi(s)$ (see *Help > Color Code*). If the operator A is a density operator, the function f is called a Wigner function.

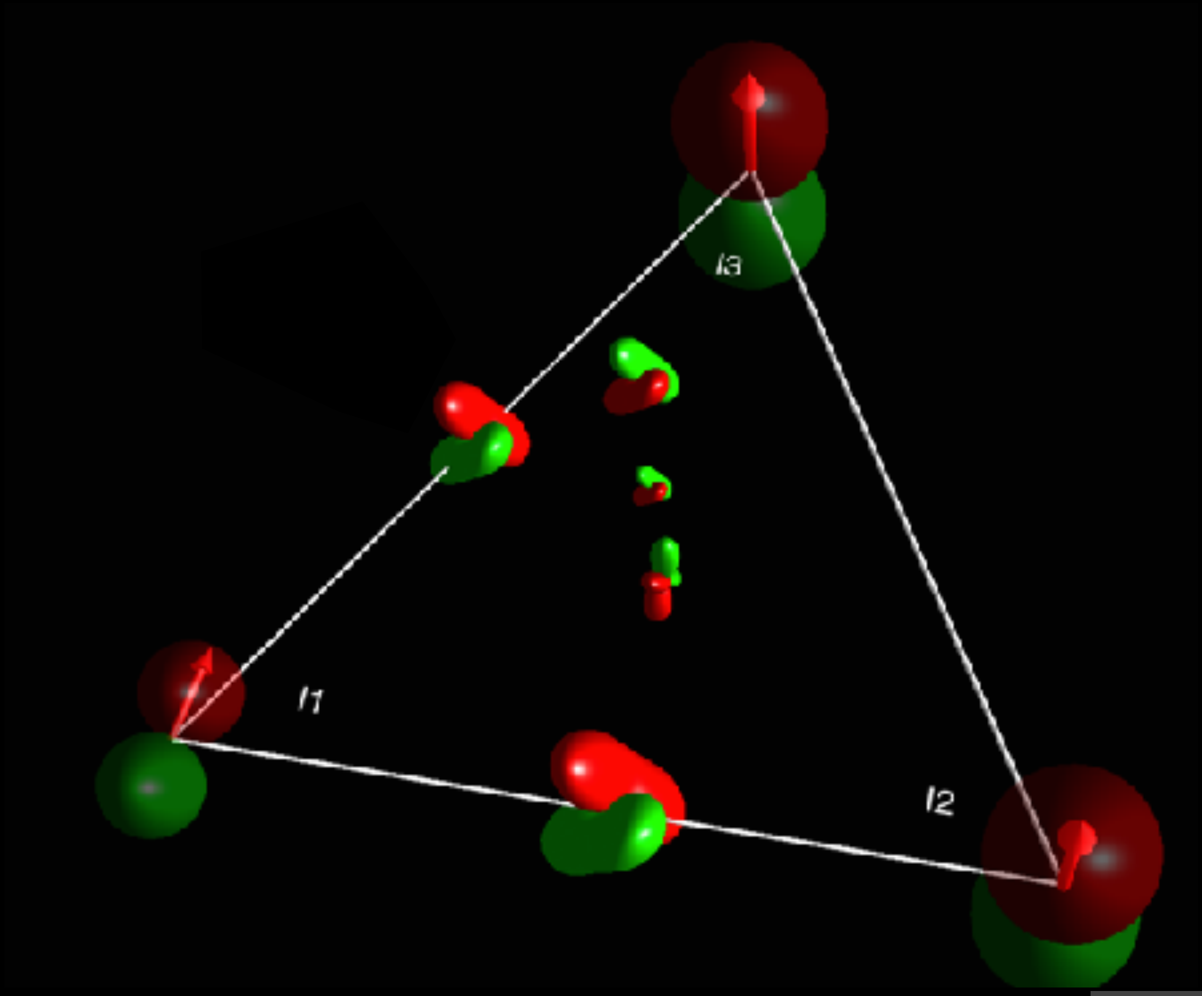
DROPS Display and Wigner Representation of Coupled Spins

For systems consisting of coupled spins, an operator A can still be expressed as a linear combination of tensor operators. However, in this case, different tensor operators with the same rank j exist, which would make the correspondence not one-to-one if they would be mapped to the same spherical harmonic Y_{jm}. This problem can be circumvented by *grouping* the tensor operators into *discrete* sets (labelled ℓ), where tensor operators with rank j appear not more than once in each set ℓ. As the tensor operators form a complete basis, any operator A can then also be decomposed in components that correspond to these discrete sets ℓ of tensor operators:

$$A = \sum_{\ell} A^{(\ell)}$$

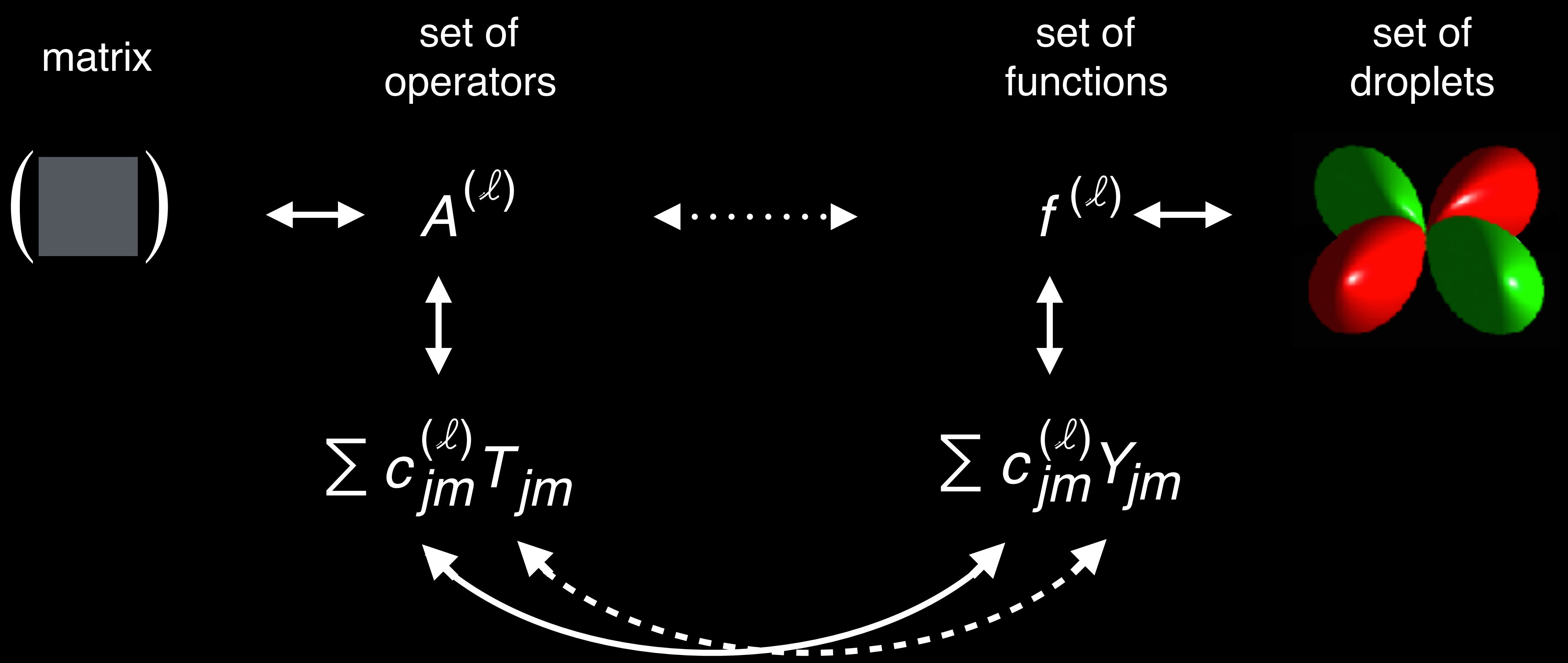
In analogy to the case of single spins, each component $A^{(\ell)}$ can be mapped to a function $f^{(\ell)}$ on a sphere and represented by a corresponding colored shape (see next page).

This is the basic idea of the **DROPS** representation of operators (where the acronym **DROPS** stands for **D**iscrete **R**epresentation of spin **OP**erator**S**) and the individual shapes are called *droplets*. If the operator A is the density operator, the corresponding set of functions $f^{(\ell)}$ forms a generalized Wigner representation.



Mapping of Operator Components $A^{(\ell)}$ to Individual Droplets

If an operator A is decomposed as described above in the form $A = \sum_{\ell} A^{(\ell)}$, then each of the operator components $A^{(\ell)}$ can be represented by a function $f^{(\ell)}$ on a sphere by mapping tensor operators T_{jm} to spherical harmonics Y_{jm} as in the case of single spins:



$A^{(\ell)}$

$f^{(\ell)}$

$\sum c_{jm}^{(\ell)} T_{jm}$

$\sum c_{jm}^{(\ell)} Y_{jm}$

LISA Basis

The grouping of tensor operators T_j into discrete sets ℓ (where a tensor operators T_j with rank j appears not more than once in each set) is not unique. Depending on the application, different approaches may be preferable. For applications with distinguishable spins, the so-called LISA basis (*Garon et al., 2015*) has a number of very favorable properties and provides an intuitive DROPS visualization to represent NMR experiments graphically. It groups tensor operators based on **Li**nearity, **S**ubsystems and **A**uxiliary criteria, such as permutation symmetry (see next page). These criteria lead to a unique grouping, which defines the tensor operators up to their algebraic signs. In the standard LISA basis, the signs are chosen such as to result in intuitive shapes (*Garon et al., 2015*). In the *SpinDrops* app, the LISA basis is used by default.

Tensor Grouping in the LISA basis (A)

In the standard LISA basis, the following criteria are used for the grouping of tensor operators into discrete sets ℓ such that each set contains not more than one tensor of the same rank *j*.

Linearity

The first criterion for the grouping of tensors is the number *k* of involved spins, which is also called the *linearity* of an operator. For three-spin systems, the linearity *k* can be 0, 1, 2, or 3. Except for *k*=0, the resulting groups still contain several tensors with the same rank *j*.

Subsystems

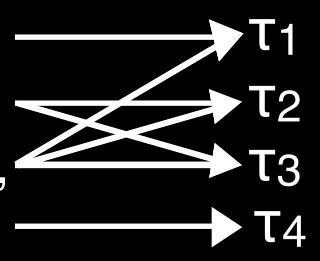
The second criterion is based on the *subset K* of spins that are involved in a tensor operator. In a system consisting of three spins, the subsets are $\{I_1\}$, $\{I_2\}$, and $\{I_3\}$ for *linear* operators (*k*=1), $\{I_1,I_2\}$, $\{I_1,I_3\}$, and $\{I_2,I_3\}$ for *bilinear* operators (*k*=2) and for each of these subsystems, not more than one tensor exists with the same rank *j*. However, this is not the case for the trilinear operators, i.e. for *trilinear* tensors involving all spins $\{I_1, I_2, I_3\}$.

Auxiliary Criteria

For k>2, auxiliary criteria are needed in order to define unique groupings of tensors. In the LISA basis, the next criterion for the grouping of tensors is based on permutation symmetry. For systems of up to five spins, this provides a unique and physically motivated grouping, such that all tensors within each group have different ranks *j*.

Tensor Grouping in the LISA basis (B)

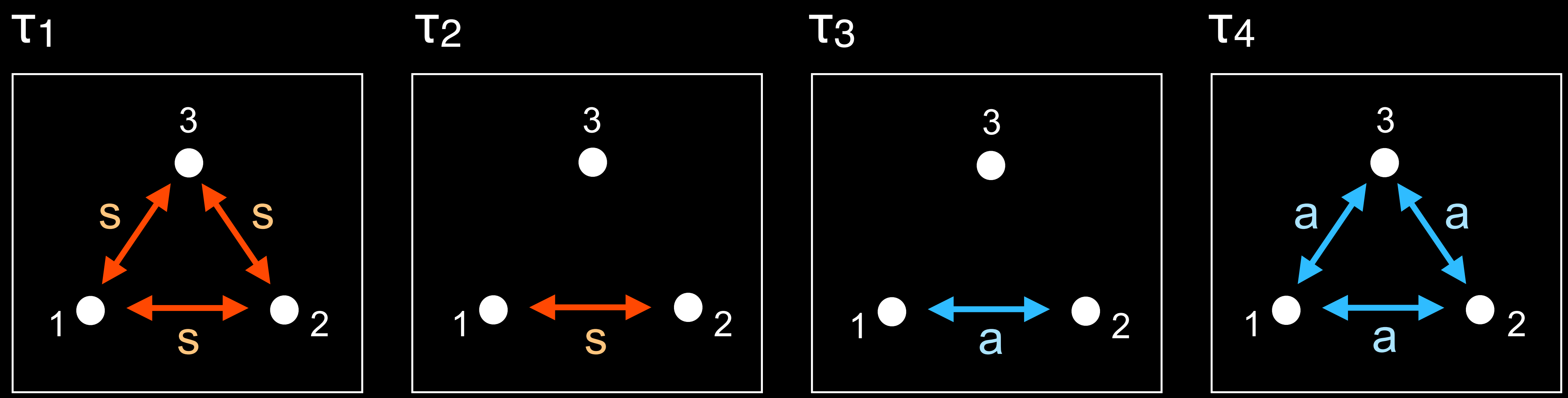
The grouping of tensors discussed on the previous page is schematically summarized below. For each linearity *k* and subsystem *K*, the rank *j* of the existing tensor operators is indicated. For the trilinear terms (*k*=3), also the permutation symmetry is indicated (in terms of so-called Young Tableaux, see *Garon et al.*, *2015*), which is used an auxiliary criterion to define sets of tensors in which all ranks *j* are different. The table also indicates the labels ℓ of the resulting unique sets of tensor operators and of the corresponding *droplets* in the DROPS representation.



Linearity k	Subsystem	Rank j	Permutation Symmetry	Label of each set ℓ
0	∅	0		Id
1	$\{I_1\}$	1		I_1
	$\{I_2\}$	1		I_2
	$\{I_3\}$	1		I_3
2	$\{I_1,I_2\}$	2,1,0		$\{I_1,I_2\}$
	$\{I_1,I_3\}$	2,1,0		$\{I_1,I_3\}$
	$\{I_2,I_3\}$	2,1,0		$\{I_2,I_3\}$
3	$\{I_1,I_2,I_3\}$	3,	τ_1	τ_1
		2,2,	τ_2	τ_2
		1,1,1,	τ_3	τ_3
		0	τ_4	τ_4

Tensor Grouping in the LISA basis (C)

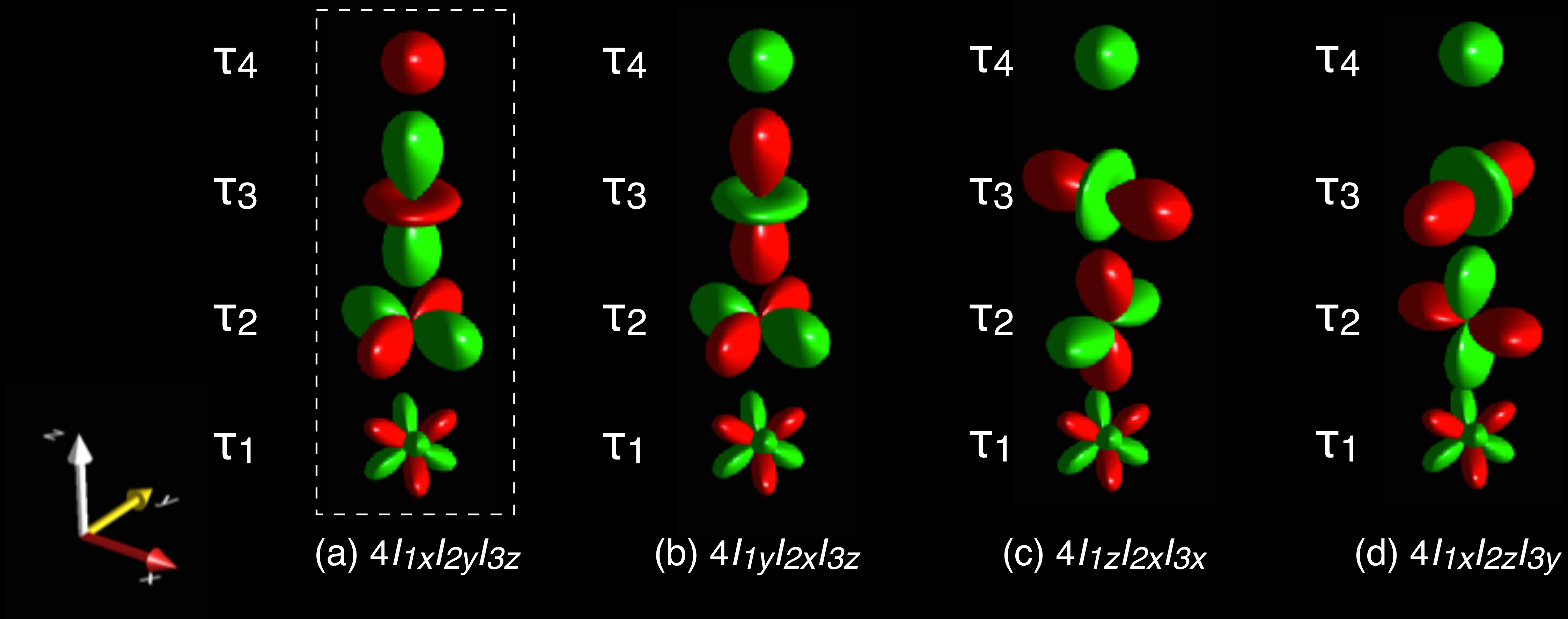
The trilinear operators corresponding to the sets τ_1, τ_2, τ_3, and τ_4 have characteristic symmetries with respect to permutations of spin labels. As illustrated schematically below, the tensor operators in set τ_1 are symmetric (s) with respect to any pairwise exchange of spin labels, i.e. any exchange of spin labels leaves these operators invariant. Conversely, the operators in set τ_4 are anti-symmetric (a) with respect to any pairwise exchange of spin labels, i.e. any exchange of spin labels changes the sign of these operators. The tensor operators in set τ_2 are symmetric (s) only with respect to the exchange of spin labels 1 and 2, whereas the tensor operators in set τ_3 are anti-symmetric (a) with respect to the exchange of spin labels 1 and 2.



This is illustrated on the following page for the decomposition of the operator $4I_{1x}I_{2y}I_{3z}$.

Tensor Grouping in the LISA basis (D)

The symmetry of the droplets τ_1, τ_2, τ_3, and τ_4 with respect to a permutation of spin labels is illustrated for the operator $4I_{1x}I_{2y}I_{3z}$ (a). Permuting spins 1 and 2 results in the operator $4I_{2x}I_{1y}I_{3z} = 4I_{1y}I_{2x}I_{3z}$ (b) and as expected, the droplets τ_1 and τ_2, which are symmetric under the (1,2) permutation, are unchanged. In contrast, the droplets τ_3 and τ_4, which are anti-symmetric with regard to this operation, change sign (resulting in inverted colors). The (1,3) permutation results in the operator $4I_{3x}I_{2y}I_{1z} = 4I_{1z}I_{2y}I_{3x}$ (c) and the (2,3) permutation results in the operator $4I_{1x}I_{3y}I_{2z} = 4I_{1x}I_{2z}I_{3y}$ (d). As discussed on the previous page, droplet τ_1 is also symmetric with respect to these permutations and is identical to case (a). Droplet τ_4 is anti-symmetric with respect to these permutations, resulting in a color change from red to green.



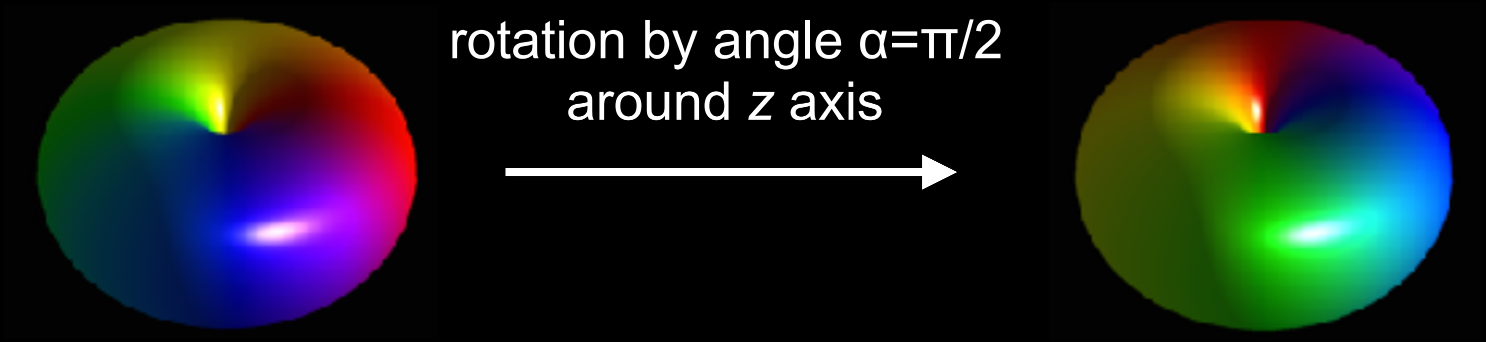
(a) $4I_{1x}I_{2y}I_{3z}$ (b) $4I_{1y}I_{2x}I_{3z}$ (c) $4I_{1z}I_{2x}I_{3x}$ (d) $4I_{1x}I_{2z}I_{3y}$

Coherence Order (A)

An operator *A* has a well-defined coherence order *p* if a rotation around the *z* axis by an arbitrary angle α reproduces the operator *A* up to an additional phase factor exp(–i*p*α), i.e. if

$$A \xrightarrow[]{\text{rotation by angle } \alpha \text{ around } z \text{ axis}} e^{-ip\alpha} A$$

Similarly, a *droplet* representing a function $f^{(\ell)}$ corresponds to an operator term $A^{(\ell)}$ with well-defined coherence order *p*, if a rotation around the *z* axis by an arbitrary angle α reproduces the *droplet* up to an additional phase factor exp(–i*p*α). For simplicity, in the following we drop the superscript "(ℓ)". For example, let us consider the rotation of the following *droplet* with p=+1 by π/2 (i.e. 90°) around the z axis:


rotation by angle α=π/2
around *z* axis

$$f(s) = r(s)\, e^{i\phi(s)}$$

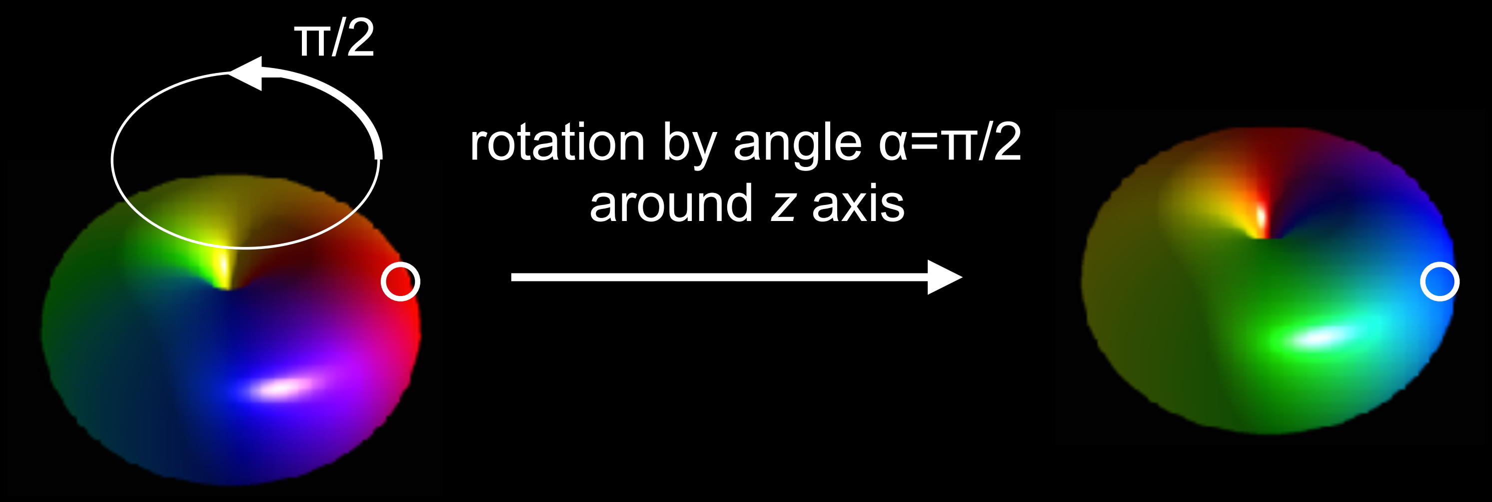
$$f'(s) = e^{-ip\alpha}\, f(s) = r(s)\, e^{i\phi'(s)}$$

with $\phi'(s) = \phi(s) - p\alpha = \phi(s) - \pi/2$

Coherence Order (B)

For a droplet with coherence order p, the corresponding function $f(s) = r(s)\, e^{i\phi(s)}$ is transformed by a z rotation with an angle α to $f'(s) = r(s)\, e^{i\phi'(s)}$ with $\phi'(s) = \phi(s) - p\alpha$.

In order to illustrate this point, consider the example shown on the previous page with p=+1 and α=π/2.



π/2

rotation by angle α=π/2
around z axis

After the rotation, the *shape* of the droplet is the same but the *color* (representing the phase of the function f) has changed. For example, the color of the point indicated by the small white circle has changed from *red* (corresponding to $\phi = 0$) to *blue* (corresponding to $\phi' = -\pi/2$), which is exactly what is expected from the general formula $\phi'(s) = \phi(s) - p\alpha = 0 - (+1)\,\pi/2$ *given above.*

Glossary of Terms and Acronyms

Glossary of Terms and Acronyms (A)

This is a summary of terms and acronyms used in *SpinDrops* and in the accompanying tutorial and help files. For an introduction to basic NMR concepts related to the dynamics of coupled spin systems, we refer to excellent books by Keeler (*Understanding Understanding NMR Spectroscopy*), Cavanagh, Fairbrother, Palmer, Skelton, Rance (*Protein NMR Spectroscopy, Principles and Practice*), Levitt (*Spin Dynamics: Basics of Nuclear Magnetic Resonance*), Ernst, Bodenhausen, Wokaun (*Principles of Nuclear Magnetic Resonance in One and Two Dimenisons*) or Goldman (*Quantum Description of High-Resolution NMR in Liquids*). For more information concerning concepts related to the DROPS representation, see *Garon et al. (2015)* and references cited therein.

Basis Operator: Just as a vector can be expressed as a unique combination of orthogonal basis vectors, any operator can be expressed as a unique combination of orthogonal basis operators. In NMR, the most widely used basis operators are Cartesian Product Operators and Spherical Tensor Operators.

Cartesian Product Operators: Products of individual spin opertators I_{kx}, I_{ky}, I_{kz}, where k is the spin label. In a three-spin system, examples of Cartesian product operators are I_{1x}, I_{2z}, I_{3y}, $2I_{1y}I_{2z}$, or $4I_{1z}I_{2z}I_{3x}$. (The prefactors 2 and 4 of the bilinear and trilinear Cartesian product operators ensure that all terms have the same norm.)

Glossary of Terms and Acronyms (B)

Complex Numbers: Recall that a complex number $c = a + ib$ can be expressed in terms of its real and imaginary parts a and b, but also in terms of their *amplitude* r and *phase* ϕ, where $r^2=a^2+b^2$ and $\tan\phi=b/a$. The amplitude r corresponds to the distance of the complex number from the origin of the complex plane. For a given *phase* ϕ, the corresponding *phase factor* is given by the complex number $\cos(\phi)+i \sin(\phi)=\exp(i\phi)$, which has an amplitude of 1 and is located on the unit circle in the complex plane.

DEPT (Distortionless Enhancement of Polarization Transfer) is a technique for heteronuclear polarization transfer and spectral editing.

Density Operator: The operator describes the state of a spin system. More precisely, it encodes the information about the state of an ensemble of spin systems and allows us to calculate experimentally relevant expectation values of observables, such as the detectable transverse magnetization of spins.

DROPS stands for **D**iscrete **R**epresentation of spin **OP**erator**S**. This is a general approach to visualize abstract quantum mechanical operators of coupled spin systems (*Garon et al., 2015*).

Droplet: In the DROPS representation, operators are mapped to a set of complex functions on a sphere. Each of these function is plotted at a different location. The shape and color of each droplet represent the orientation-dependent amplitude and phase of the complex function, respectively.

E represents the identity operator.

Glossary of Terms and Acronyms (C)

Hamilton Operator (or **Hamiltonian**): The quantum mechanical operator that corresponds to the energy of a spin system. It includes terms for frequency offsets, couplings and pulses.

Hermitian Operator (Self-Adjoint Operator): *Hermitian* operators play an important role in quantum mechanics as they have real eigenvalues and expectation values. Observables correspond to Hermitian operators. Cartesian product operators are Hermitian. Any Hermitian operator can be expressed as a linear combination of Cartesian product operators with real coefficients. The multiplication of a Hermitian operator by i results in a *skew-Hermitian* operator.

I1, I2, I3 denote the first (I_1), second (I_2), and third (I_3) spin in a spin system.

INEPT stands for **I**nsensitive **N**uclei **E**nhanced by **P**olarization **T**ransfer

Linearity: The linearity of an operator reflects the number of involved single-spin operators. For example, I_{1x}, $2I_{1x}I_{2y}$ and $4I_{1x}I_{2z}I_{3y}$ are linear, bilinear and trilinear operators, respectively.

LISA: A tensor basis which is defined based on **Li**nearity, **S**ubsystems and **A**uxiliary criteria. In addition to the number of involved spins (linearity) and the subset of involved spins (subsystem), permutation symmetry provides a sufficient auxiliary criterion to uniquely define the tensor basis (up to algebraic signs) for systems consisting of up to five spins 1/2. Additional criteria are necessary for more than five spins. For a rigorous definition, see *Garon et al. (2015)*.

Glossary of Terms and Acronyms (D)

Phase: The term *phase* typically refers to the argument of a periodic function. This term can be somewhat confusing because it appears in different contexts in NMR, where it is associated with different properties.

In the context of *pulses*, the *phase* corresponds to the transverse rotation axis in the rotating frame. It can be defined in terms of the *angle* between the x axis and the rotation axis (in units of degree, e.g. 90° or in units of radians, e.g. $\pi/2$) or by the rotation axis itself (e.g. y).

In the context of *complex numbers,* the *phase* refers to the angle between the real axis and the line between the origin and the location of a given complex number in the complex plane.

The relation between z rotations and *phase factors* of *operators* plays an important role in the definition of *coherence order*. In the DROPS representation, individual *droplets* represent complex functions on a sphere, where the orientation-dependent phase of each complex function is represented graphically by colors.

Tensor Operators: An irreducible spherical tensor T_j with rank j has $2j+1$ *components* T_{jm} with *order* $m \in \{-j, \dots, j\}$. The operators T_{jm} form a basis of a space which stays invariant under rotations. In the Condon-Shortley phase convention, only the operators T_{j0} (with order 0) are Hermitian. Tensor operators form an ideal basis for the DROPS representation because of their favorable properties under non-selective rotations and their close relationship with spherical harmonics Y_{jm}.

Glossary of Terms and Acronyms (E)

TOCSY (Total Correlation Spectroscopy) is based on the efficient transfer of polarization or coherence between coupled spins under isotropic mixing conditions. Isotropic mixing conditions can be created by TOCSY multiple-pulse sequences. In homonuclear spin systems, the effective coupling constants of the isotropic mixing Hamiltonian are ideally identical to the actual couplings between the spins. For the simple case of two coupled spins 1/2, polarization or coherence can be transferred from one spin to the other spin, resulting in cross peaks in two-dimensional TOCSY experiments. The optimal mixing time is $t=1/(J_{12})$. For systems consisting of more than two spins 1/2, polarization and coherence is transferred between all spins of a coupling network, resulting in „total correlation“ spectra. (Isotropic mixing conditions can also be created in heteronuclear spin systems, but the effective coupling constants of the isotropic mixing Hamiltonian are scaled down to 1/3 of the actual couplings between the spins).

Acknowledgements

References and Acknowledgements

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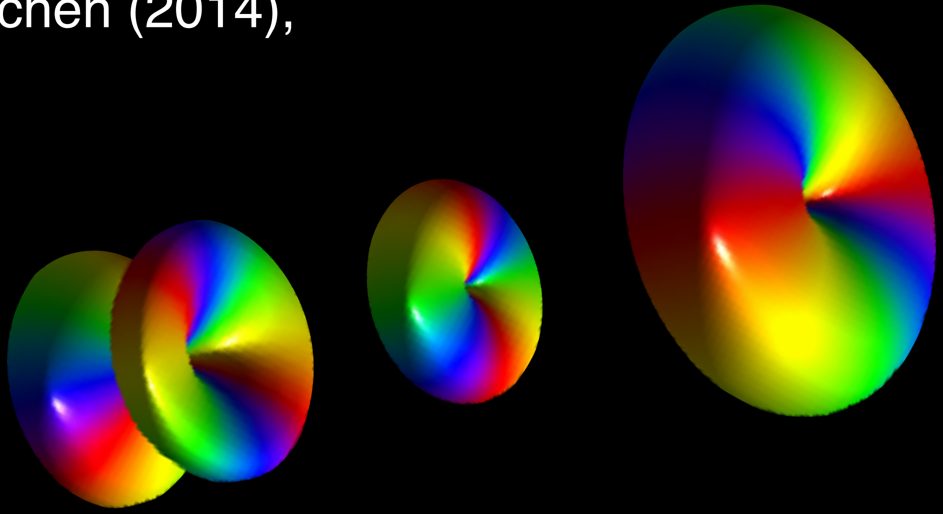

Related work:

The DROPS representation of coupled spins can be viewed as a generalized Wigner function and builds on previous ideas by many researchers, including E. Wigner, J. E. Moyal, R.L. Stratanovich, A. Pines, S. Vega, D. Wemmer, T.K. Halstead, B.C. Sanctuary, J. C. Várrily, J. M. Garcia-Bondia, F.P. Temme, J. Listerud, G.P. Drobny, G.S. Agarval, W.P. Schleich, J. P. Dowling, S. Brif, A. Mann, P.W. Kuchel, P.S. Jessen, I.H. Deutsch and many others. For a more complete account and detailed references to related work, please see *Garon et al. (2015)*.

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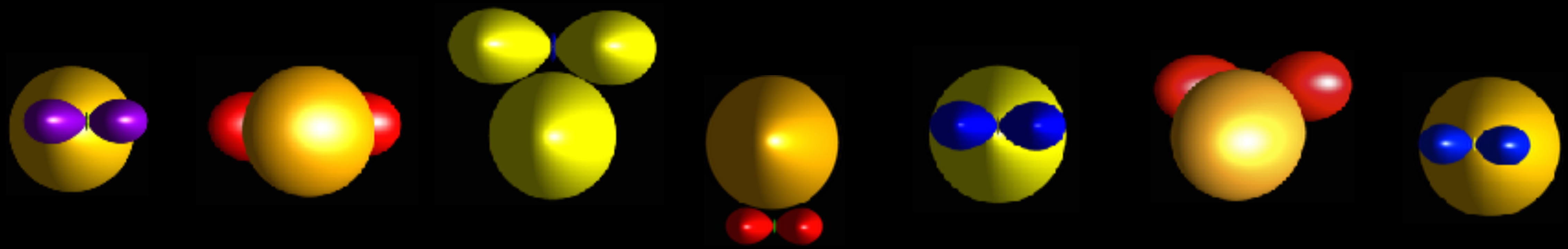

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