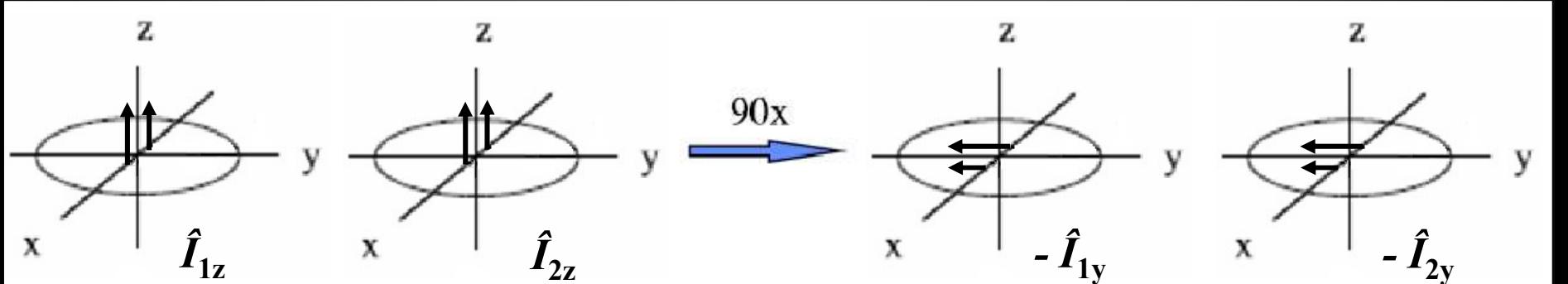


# COSY

## Product operator formalism:

$$\pi/2 - t_1 - \pi/2 - t_2 \text{ (acquisition)}$$

**1<sup>st</sup> stage: 1<sup>st</sup> 90°<sub>x</sub>**       $\hat{I}_{1z} + \hat{I}_{2z} \xrightarrow{\pi/2_x} -\hat{I}_{1y} - \hat{I}_{2y}$



# COSY

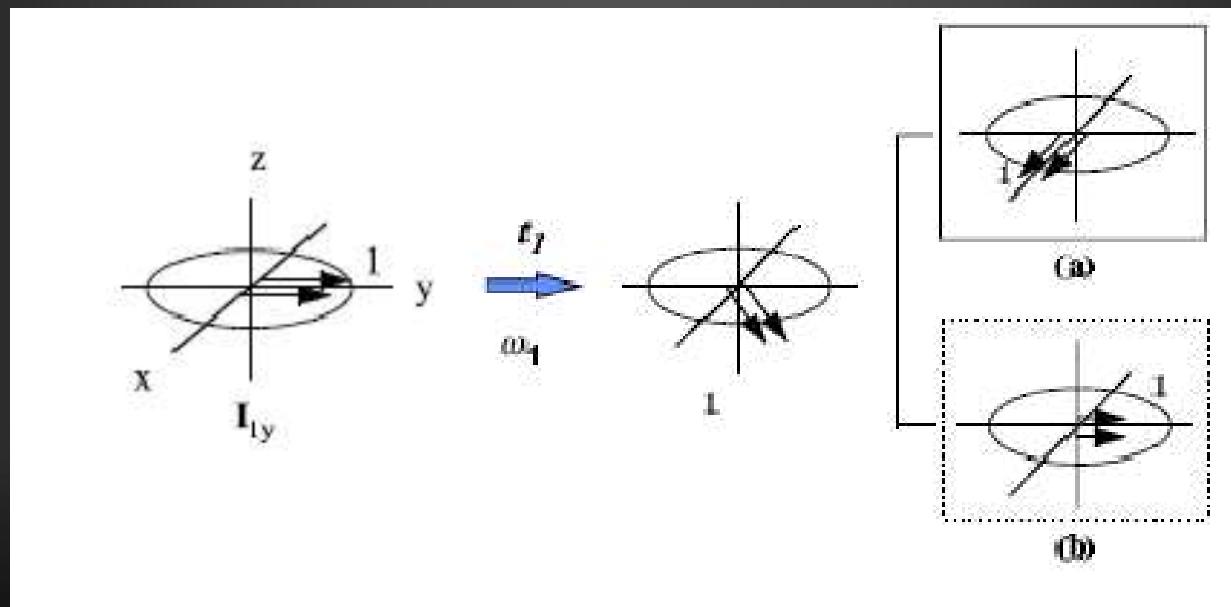
## Product operator formalism:

**2<sup>nd</sup> stage: chemical shift**

( $\Omega$ ) and ( $J$ ) evolution at  $t_1$

$$- \hat{I}_{1y} \xrightarrow{-\hat{I}_{1y}} -\hat{I}_{2y} \xrightarrow{\Omega_1 t_1 \hat{I}_{1z} + \Omega_2 t_1 \hat{I}_{2z}}$$

$$- \hat{I}_{1y} \cos(\Omega_1 t_1) + \hat{I}_{1x} \sin(\Omega_1 t_1)$$



# COSY

## Product operator formalism:

**2<sup>nd</sup> stage: chemical shift**

( $\Omega$ ) and ( $J$ ) **evolution at  $t_1$**

$$- \hat{I}_{1y} - \hat{I}_{2y} \xrightarrow{\Omega_1 t_1 \hat{I}_{1z} + \Omega_2 t_1 \hat{I}_{2z}}$$

$$- \hat{I}_{1y} \cos(\Omega_1 t_1) + \hat{I}_{1x} \sin(\Omega_1 t_1) - \hat{I}_{2y} \cos(\Omega_2 t_1) + \hat{I}_{2x} \sin(\Omega_2 t_1)$$

# COSY

## Product operator formalism:

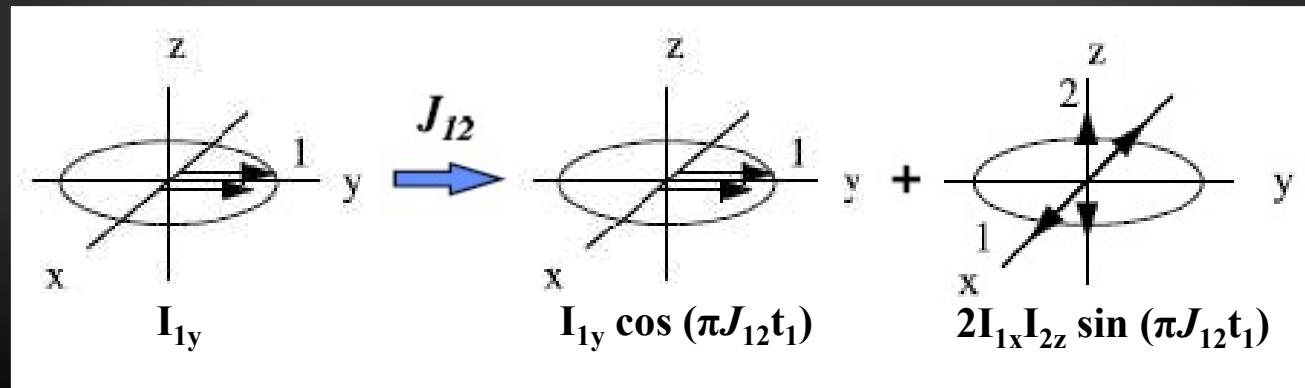
***2<sup>nd</sup> stage: chemical shift***

**( $\Omega$ ) and ( $J$ ) evolution at  $t_1$**

$$- \hat{I}_{1y} \cos(\Omega_1 t_1) + \hat{I}_{1x} \sin(\Omega_1 t_1) - \hat{I}_{2y} \cos(\Omega_2 t_1) + \hat{I}_{2x} \sin(\Omega_2 t_1)$$

$$\frac{\pi J_{12} t_1 2(\hat{I}_{1z} \hat{I}_{2z})}{\longrightarrow}$$

$$- \hat{I}_{1y} \cos(\Omega_1 t_1) \cos(\pi J_{12} t_1) + 2 \hat{I}_{1x} \hat{I}_{2z} \cos(\Omega_1 t_1) \sin(\pi J_{12} t_1)$$



# COSY

## Product operator formalism:

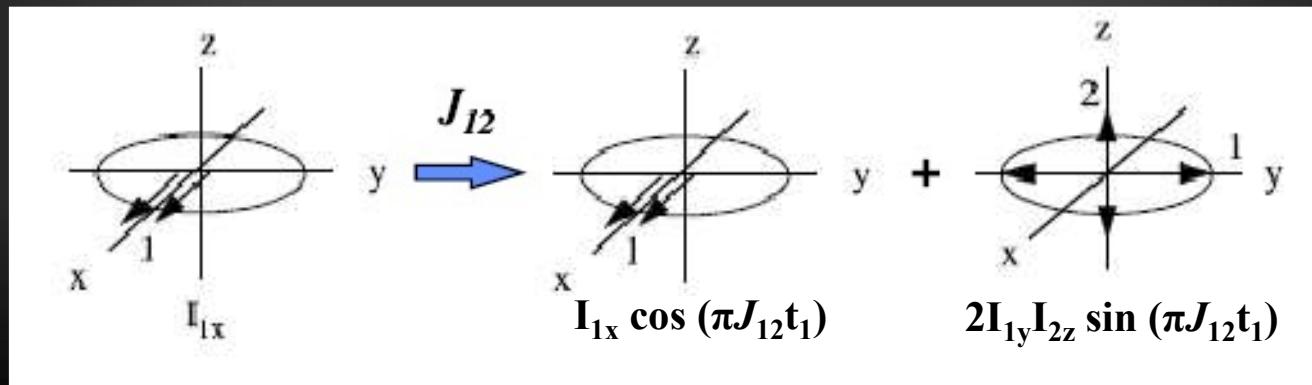
***2<sup>nd</sup> stage: chemical shift***

**( $\Omega$ ) and ( $J$ ) evolution at  $t_1$**

$$- \hat{I}_{1y} \cos(\Omega_1 t_1) + \boxed{\hat{I}_{1x} \sin(\Omega_1 t_1)} - \hat{I}_{2y} \cos(\Omega_2 t_1) + \hat{I}_{2x} \sin(\Omega_2 t_1)$$

$$\xrightarrow{\pi J_{12} t_1 2(\hat{I}_{1z} \hat{I}_{2z})}$$

$$+ \hat{I}_{1x} \sin(\Omega_1 t_1) \cos(\pi J_{12} t_1) + 2 \hat{I}_{1y} \hat{I}_{2z} \sin(\Omega_1 t_1) \sin(\pi J_{12} t_1)$$



# COSY

## Product operator formalism:

***2<sup>nd</sup> stage: chemical shift***

***(Ω) and (J) evolution in  $t_1$***

$$- \hat{I}_{1y} \cos(\Omega_1 t_1) + \hat{I}_{1x} \sin(\Omega_1 t_1) - \hat{I}_{2y} \cos(\Omega_2 t_1) + \hat{I}_{2x} \sin(\Omega_2 t_1)$$

$$\xrightarrow{\pi J_{12} t_1 2(\hat{I}_{1z} \hat{I}_{2z})}$$

$$- \hat{I}_{1y} \cos(\Omega_1 t_1) \cos(\pi J_{12} t_1) + 2 \hat{I}_{1x} \hat{I}_{2z} \cos(\Omega_1 t_1) \sin(\pi J_{12} t_1)$$

$$+ \hat{I}_{1x} \sin(\Omega_1 t_1) \cos(\pi J_{12} t_1) + 2 \hat{I}_{1y} \hat{I}_{2z} \sin(\Omega_1 t_1) \sin(\pi J_{12} t_1)$$

$$- \hat{I}_{2y} \cos(\Omega_2 t_1) \cos(\pi J_{12} t_1) + 2 \hat{I}_{1z} \hat{I}_{2x} \cos(\Omega_2 t_1) \sin(\pi J_{12} t_1)$$

$$+ \hat{I}_{2x} \sin(\Omega_2 t_1) \cos(\pi J_{12} t_1) + 2 \hat{I}_{1z} \hat{I}_{2y} \sin(\Omega_2 t_1) \sin(\pi J_{12} t_1)$$

# COSY

## Product operator formalism:

$$- \hat{I}_{1y} \cos(\Omega_1 t_1) \cos(\pi J_{12} t_1) + 2 \hat{I}_{1x} \hat{I}_{2z} \cos(\Omega_1 t_1) \sin(\pi J_{12} t_1)$$

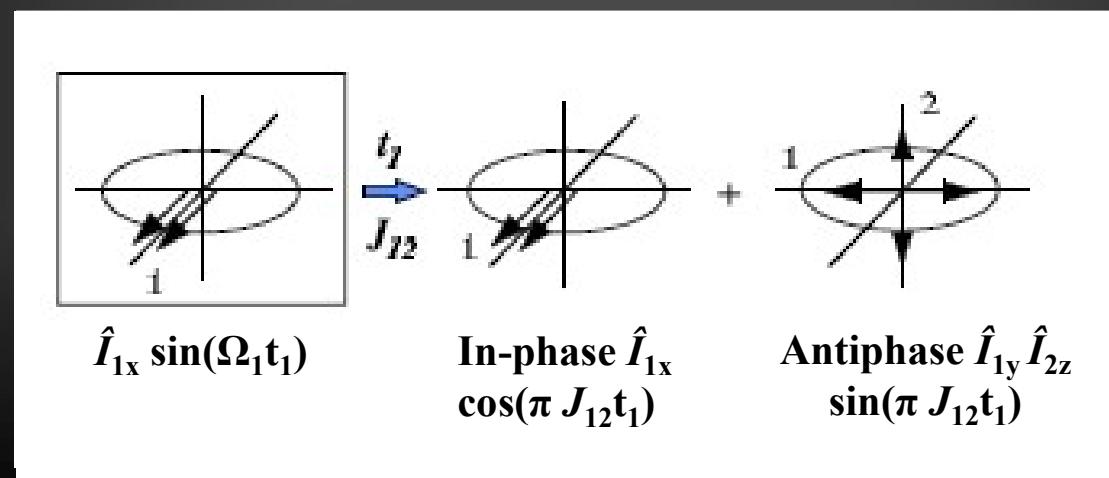
$$+ \hat{I}_{1x} \sin(\Omega_1 t_1) \cos(\pi J_{12} t_1) + 2 \hat{I}_{1y} \hat{I}_{2z} \sin(\Omega_1 t_1) \sin(\pi J_{12} t_1)$$

$$- \hat{I}_{2y} \cos(\Omega_2 t_1) \cos(\pi J_{12} t_1) + 2 \hat{I}_{1z} \hat{I}_{2x} \cos(\Omega_2 t_1) \sin(\pi J_{12} t_1)$$

$$+ \hat{I}_{2x} \sin(\Omega_2 t_1) \cos(\pi J_{12} t_1) + 2 \hat{I}_{1z} \hat{I}_{2y} \sin(\Omega_2 t_1) \sin(\pi J_{12} t_1)$$

In-phase single-quantum

antiphase single-quantum



# COSY

## Product operator formalism:

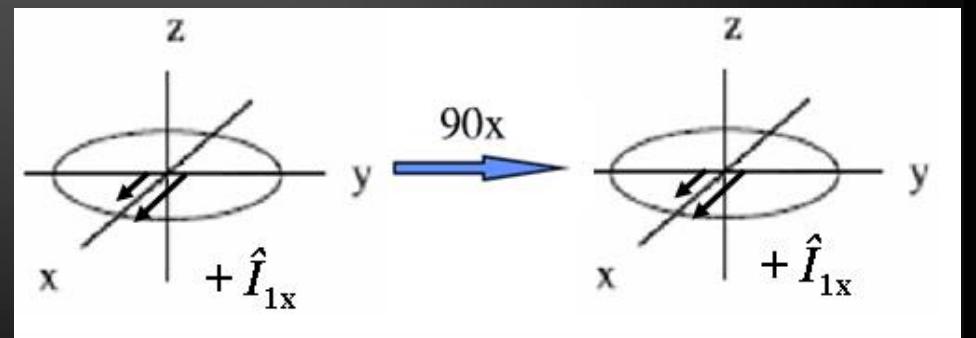
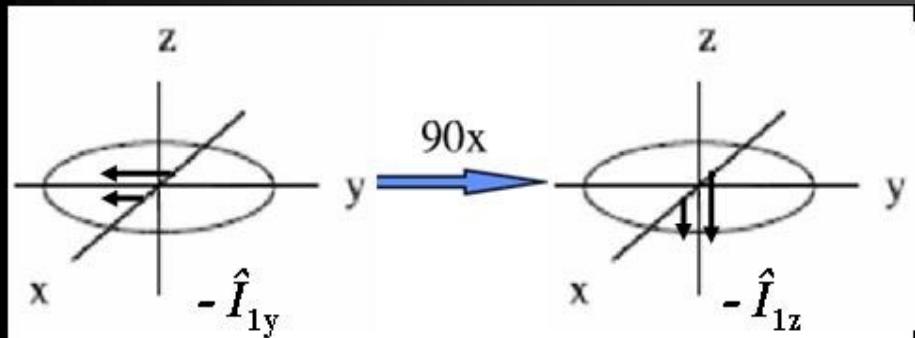
$$- \hat{I}_{1y} \cos(\Omega_1 t_1) \cos(\pi J_{12} t_1) + 2 \hat{I}_{1x} \hat{I}_{2z} \cos(\Omega_1 t_1) \sin(\pi J_{12} t_1)$$

$$+ \hat{I}_{1x} \sin(\Omega_1 t_1) \cos(\pi J_{12} t_1) + 2 \hat{I}_{1y} \hat{I}_{2z} \sin(\Omega_1 t_1) \sin(\pi J_{12} t_1)$$

$$- \hat{I}_{2y} \cos(\Omega_2 t_1) \cos(\pi J_{12} t_1) + 2 \hat{I}_{1z} \hat{I}_{2x} \cos(\Omega_2 t_1) \sin(\pi J_{12} t_1)$$

$$+ \hat{I}_{2x} \sin(\Omega_2 t_1) \cos(\pi J_{12} t_1) + 2 \hat{I}_{1z} \hat{I}_{2y} \sin(\Omega_2 t_1) \sin(\pi J_{12} t_1)$$

3<sup>rd</sup> stage: 2<sup>nd</sup> 90°<sub>x</sub>  $\xrightarrow{\pi/2_x}$



$$- \hat{I}_{1z} \cos(\Omega_1 t_1) \cos(\pi J_{12} t_1)$$

$$+ \hat{I}_{1x} \sin(\Omega_1 t_1) \cos(\pi J_{12} t_1)$$

# COSY

## Product operator formalism:

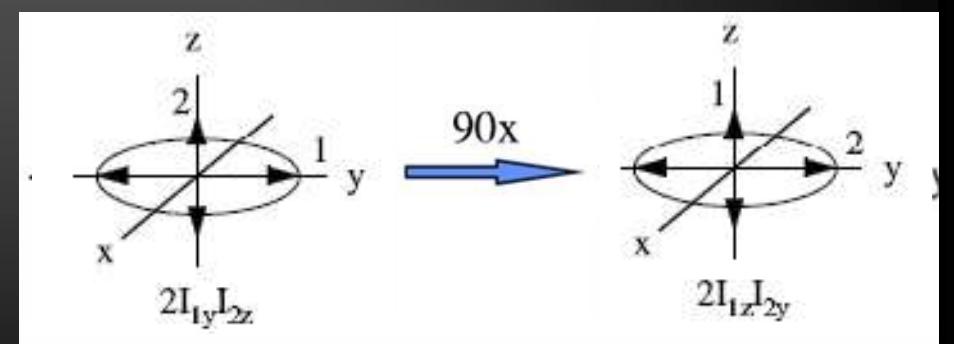
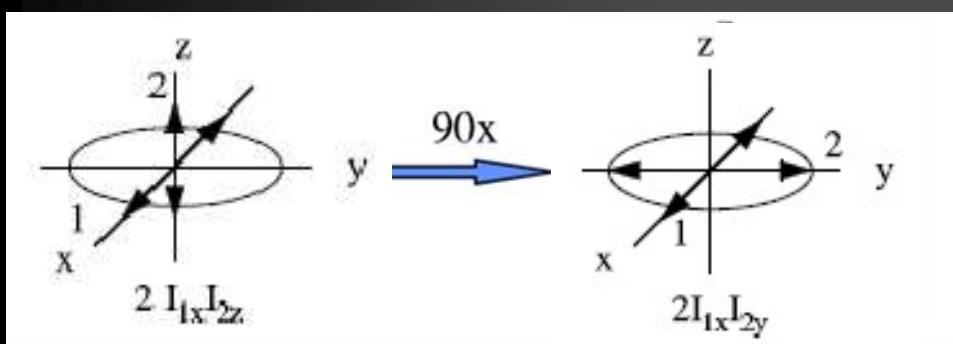
$$- \hat{I}_{1y} \cos(\Omega_1 t_1) \cos(\pi J_{12} t_1) + 2 \hat{I}_{1x} \hat{I}_{2z} \cos(\Omega_1 t_1) \sin(\pi J_{12} t_1)$$

$$+ \hat{I}_{1x} \sin(\Omega_1 t_1) \cos(\pi J_{12} t_1) + 2 \hat{I}_{1y} \hat{I}_{2z} \sin(\Omega_1 t_1) \sin(\pi J_{12} t_1)$$

$$- \hat{I}_{2y} \cos(\Omega_2 t_1) \cos(\pi J_{12} t_1) + 2 \hat{I}_{1z} \hat{I}_{2x} \cos(\Omega_2 t_1) \sin(\pi J_{12} t_1)$$

$$+ \hat{I}_{2x} \sin(\Omega_2 t_1) \cos(\pi J_{12} t_1) + 2 \hat{I}_{1z} \hat{I}_{2y} \sin(\Omega_2 t_1) \sin(\pi J_{12} t_1)$$

**3<sup>rd</sup> stage: 2<sup>nd</sup> 90°<sub>x</sub>     $\pi/2$  <sub>x</sub>**



$$- 2 \hat{I}_{1x} \hat{I}_{2y} \cos(\Omega_1 t_1) \sin(\pi J_{12} t_1)$$

$$- 2 \hat{I}_{1z} \hat{I}_{2y} \cos(\Omega_1 t_1) \sin(\pi J_{12} t_1)$$

# COSY

## Product operator formalism:

$$\begin{aligned} & - \hat{I}_{1y} \cos(\Omega_1 t_1) \cos(\pi J_{12} t_1) + 2 \hat{I}_{1x} \hat{I}_{2z} \cos(\Omega_1 t_1) \sin(\pi J_{12} t_1) \\ & + \hat{I}_{1x} \sin(\Omega_1 t_1) \cos(\pi J_{12} t_1) + 2 \hat{I}_{1y} \hat{I}_{2z} \sin(\Omega_1 t_1) \sin(\pi J_{12} t_1) \\ & - \hat{I}_{2y} \cos(\Omega_2 t_1) \cos(\pi J_{12} t_1) + 2 \hat{I}_{1z} \hat{I}_{2x} \cos(\Omega_2 t_1) \sin(\pi J_{12} t_1) \\ & + \hat{I}_{2x} \sin(\Omega_2 t_1) \cos(\pi J_{12} t_1) + 2 \hat{I}_{1z} \hat{I}_{2y} \sin(\Omega_2 t_1) \sin(\pi J_{12} t_1) \end{aligned}$$

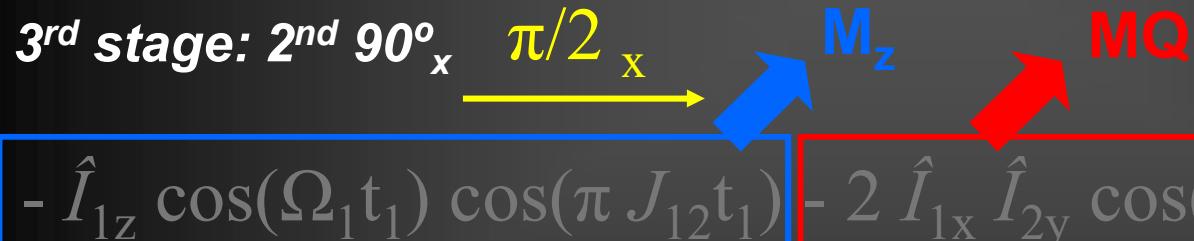
**3<sup>rd</sup> stage: 2<sup>nd</sup> 90°<sub>x</sub>**  $\xrightarrow{\pi/2_x}$

$$\begin{aligned} & - \hat{I}_{1z} \cos(\Omega_1 t_1) \cos(\pi J_{12} t_1) - 2 \hat{I}_{1x} \hat{I}_{2y} \cos(\Omega_1 t_1) \sin(\pi J_{12} t_1) \\ & + \hat{I}_{1x} \sin(\Omega_1 t_1) \cos(\pi J_{12} t_1) - 2 \hat{I}_{1z} \hat{I}_{2y} \sin(\Omega_1 t_1) \sin(\pi J_{12} t_1) \\ & - \hat{I}_{2z} \cos(\Omega_2 t_1) \cos(\pi J_{12} t_1) - 2 \hat{I}_{1y} \hat{I}_{2x} \cos(\Omega_2 t_1) \sin(\pi J_{12} t_1) \\ & + \hat{I}_{2x} \sin(\Omega_2 t_1) \cos(\pi J_{12} t_1) - 2 \hat{I}_{1y} \hat{I}_{2z} \sin(\Omega_2 t_1) \sin(\pi J_{12} t_1) \end{aligned}$$

# COSY

## Product operator formalism:

$$\begin{aligned} & -\hat{I}_{1y} \cos(\Omega_1 t_1) \cos(\pi J_{12} t_1) + 2 \hat{I}_{1x} \hat{I}_{2z} \cos(\Omega_1 t_1) \sin(\pi J_{12} t_1) \\ & + \hat{I}_{1x} \sin(\Omega_1 t_1) \cos(\pi J_{12} t_1) + 2 \hat{I}_{1y} \hat{I}_{2z} \sin(\Omega_1 t_1) \sin(\pi J_{12} t_1) \\ & - \hat{I}_{2y} \cos(\Omega_2 t_1) \cos(\pi J_{12} t_1) + 2 \hat{I}_{1z} \hat{I}_{2x} \cos(\Omega_2 t_1) \sin(\pi J_{12} t_1) \\ & + \hat{I}_{2x} \sin(\Omega_2 t_1) \cos(\pi J_{12} t_1) + 2 \hat{I}_{1z} \hat{I}_{2y} \sin(\Omega_2 t_1) \sin(\pi J_{12} t_1) \end{aligned}$$



$$\begin{aligned} & \boxed{-\hat{I}_{1z} \cos(\Omega_1 t_1) \cos(\pi J_{12} t_1)} \quad \boxed{-2 \hat{I}_{1x} \hat{I}_{2y} \cos(\Omega_1 t_1) \sin(\pi J_{12} t_1)} \\ & + \hat{I}_{1x} \sin(\Omega_1 t_1) \cos(\pi J_{12} t_1) - 2 \hat{I}_{1z} \hat{I}_{2y} \sin(\Omega_1 t_1) \sin(\pi J_{12} t_1) \\ & \boxed{-\hat{I}_{2z} \cos(\Omega_2 t_1) \cos(\pi J_{12} t_1)} \quad \boxed{-2 \hat{I}_{1y} \hat{I}_{2x} \cos(\Omega_2 t_1) \sin(\pi J_{12} t_1)} \\ & + \hat{I}_{2x} \sin(\Omega_2 t_1) \cos(\pi J_{12} t_1) - 2 \hat{I}_{1y} \hat{I}_{2z} \sin(\Omega_2 t_1) \sin(\pi J_{12} t_1) \end{aligned}$$

# COSY

## Product operator formalism:

$$+ \hat{I}_{1x} \sin(\Omega_1 t_1) \cos(\pi J_{12} t_1) - 2 \hat{I}_{1z} \hat{I}_{2y} \sin(\Omega_1 t_1) \sin(\pi J_{12} t_1)$$
$$+ \hat{I}_{2x} \sin(\Omega_2 t_1) \cos(\pi J_{12} t_1) - 2 \hat{I}_{1y} \hat{I}_{2z} \sin(\Omega_2 t_1) \sin(\pi J_{12} t_1)$$

**4<sup>th</sup> stage (acquisition): *chemical shift* ( $\Omega$ ) and ( $J$ ) evolution at  $t_2$**

$$\xrightarrow{\Omega_1 t_2 \hat{I}_{1z} + \Omega_2 t_2 \hat{I}_{2z}}$$

$$\xrightarrow{\pi J_{12} t_2 2(\hat{I}_{1z} \hat{I}_{2z})}$$

# COSY

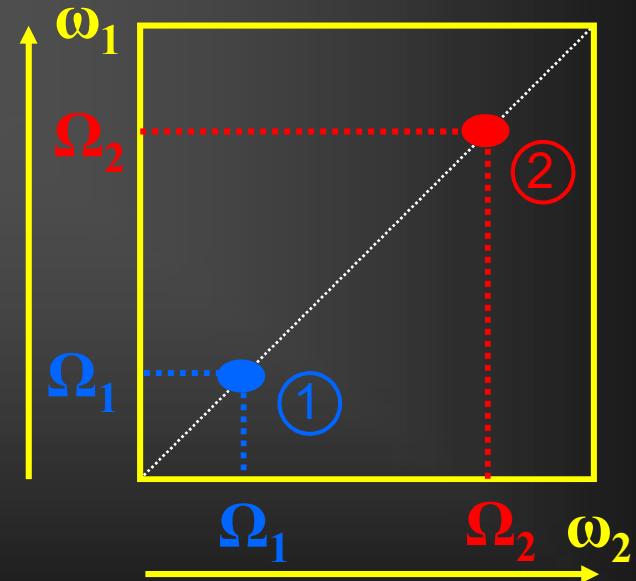
## Product operator formalism:

$$+ \hat{I}_{1x} \sin(\Omega_1 t_1) \cos(\pi J_{12} t_1) - 2 \hat{I}_{1z} \hat{I}_{2y} \sin(\Omega_1 t_1) \sin(\pi J_{12} t_1)$$
$$+ \hat{I}_{2x} \sin(\Omega_2 t_1) \cos(\pi J_{12} t_1) - 2 \hat{I}_{1y} \hat{I}_{2z} \sin(\Omega_2 t_1) \sin(\pi J_{12} t_1)$$

### **Conclusions:**

- ①  $\Omega_1$  at  $t_1$  &  $\Omega_1$  at  $t_2$
- ②  $\Omega_2$  at  $t_1$  &  $\Omega_2$  at  $t_2$

 Diagonal peaks



# COSY

## Product operator formalism:

$$+ \hat{I}_{1x} \sin(\Omega_1 t_1) \cos(\pi J_{12} t_1) - 2 \hat{I}_{1z} \hat{I}_{2y} \sin(\Omega_1 t_1) \sin(\pi J_{12} t_1)$$
$$+ \hat{I}_{2x} \sin(\Omega_2 t_1) \cos(\pi J_{12} t_1) - 2 \hat{I}_{1y} \hat{I}_{2z} \sin(\Omega_2 t_1) \sin(\pi J_{12} t_1)$$

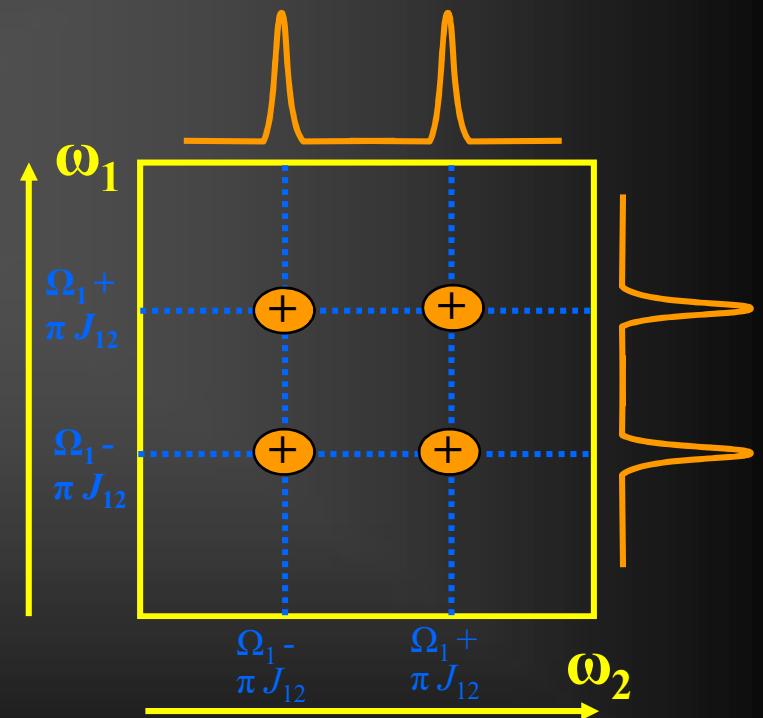
### Conclusions:

①  $\Omega_1 \text{ em } t_1 \text{ e } \Omega_1 \text{ em } t_2$

 Diagonal peak

$$+ \hat{I}_{12x} \sin(\Omega_1 t_1) \cos(\pi J_{12} t_1)$$

 Multiplet “In-phase”



# COSY

## Product operator formalism:

$$+ \hat{I}_{1x} \sin(\Omega_1 t_1) \cos(\pi J_{12} t_1) - 2 \hat{I}_{1z} \hat{I}_{2y} \sin(\Omega_1 t_1) \sin(\pi J_{12} t_1)$$
$$+ \hat{I}_{2x} \sin(\Omega_2 t_1) \cos(\pi J_{12} t_1) - 2 \hat{I}_{1y} \hat{I}_{2z} \sin(\Omega_2 t_1) \sin(\pi J_{12} t_1)$$

**Conclusions:**

①  $\Omega_1$  at  $t_1$  &  $\Omega_1$  at  $t_2$



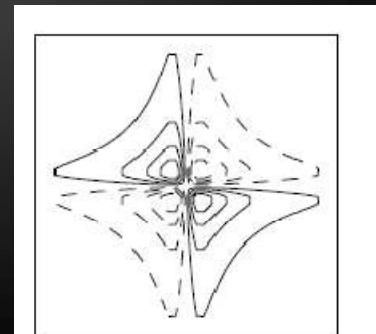
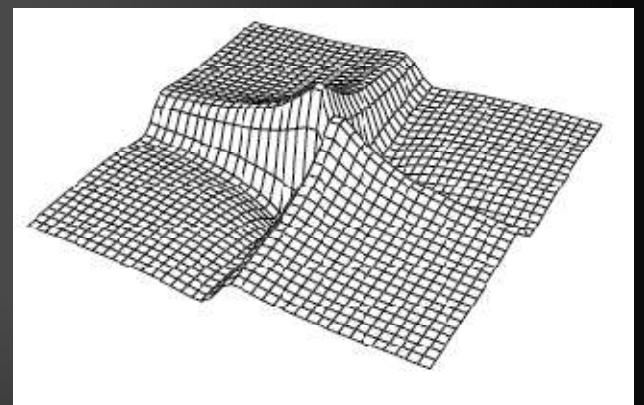
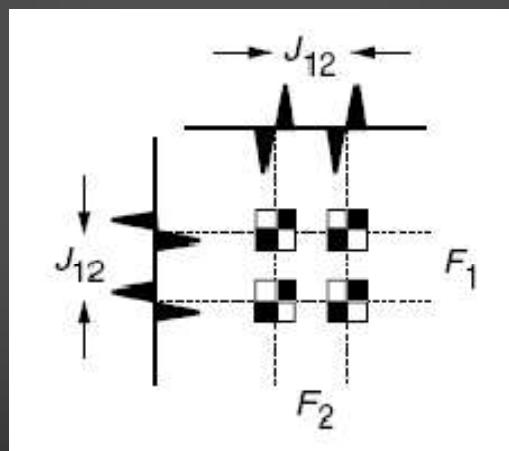
Diagonal peaks

$$+ \hat{I}_{12x} \sin(\Omega_1 t_1) \cos(\pi J_{12} t_1)$$



$$\frac{1}{2} [\sin(\Omega_1 t_1 + \pi J_{12} t_1) + \sin(\Omega_1 t_1 - \pi J_{12} t_1)]$$

Doubly dispersive



# COSY

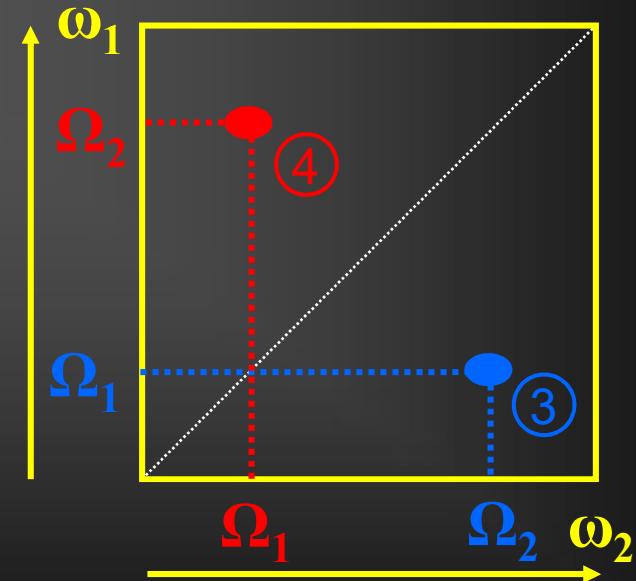
## Product operator formalism:

$$+ \hat{I}_{1x} \sin(\Omega_1 t_1) \cos(\pi J_{12} t_1) - 2 \hat{I}_{1z} \hat{I}_{2y} \sin(\Omega_1 t_1) \sin(\pi J_{12} t_1)$$
$$+ \hat{I}_{2x} \sin(\Omega_2 t_1) \cos(\pi J_{12} t_1) - 2 \hat{I}_{1y} \hat{I}_{2z} \sin(\Omega_2 t_1) \sin(\pi J_{12} t_1)$$

### Conclusions:

- ③  $\Omega_1$  at  $t_1$  &  $\Omega_2$  at  $t_2$
- ④  $\Omega_2$  at  $t_1$  &  $\Omega_1$  at  $t_2$

Cross-peaks



# COSY

## Product operator formalism:

$$+ \hat{I}_{1x} \sin(\Omega_1 t_1) \cos(\pi J_{12} t_1) - 2 \hat{I}_{1z} \hat{I}_{2y} \sin(\Omega_1 t_1) \sin(\pi J_{12} t_1)$$
$$+ \hat{I}_{2x} \sin(\Omega_2 t_1) \cos(\pi J_{12} t_1) - 2 \hat{I}_{1y} \hat{I}_{2z} \sin(\Omega_2 t_1) \sin(\pi J_{12} t_1)$$

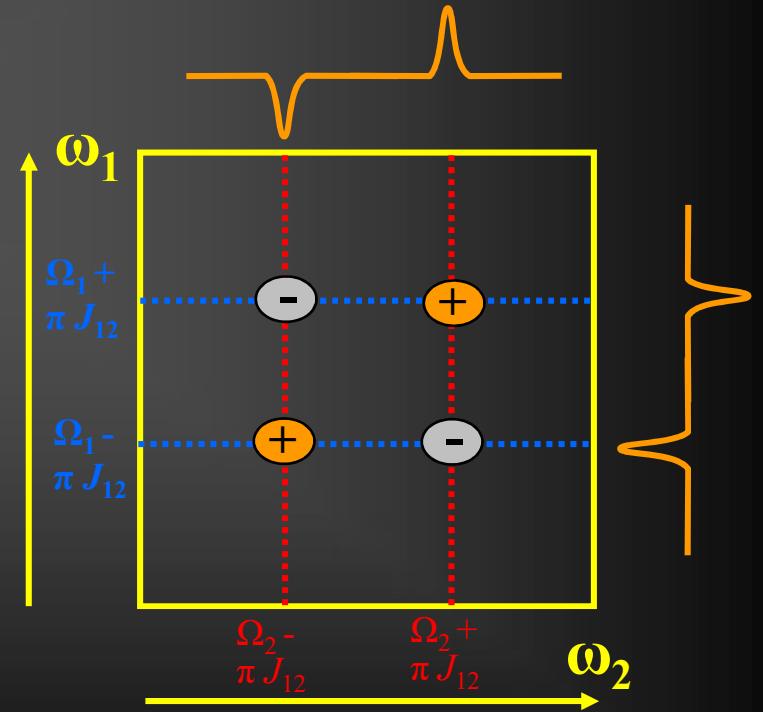
### Conclusions:

③  $\Omega_1$  at  $t_1$  &  $\Omega_2$  at  $t_2$

 Cross-peak

-  $2 \hat{I}_{1z} \hat{I}_{2y} \sin(\Omega_1 t_1) \sin(\pi J_{12} t_1)$

 Multiplet “Antiphase”



# COSY

## Product operator formalism:

$$+ \hat{I}_{1x} \sin(\Omega_1 t_1) \cos(\pi J_{12} t_1) - 2 \hat{I}_{1z} \hat{I}_{2y} \sin(\Omega_1 t_1) \sin(\pi J_{12} t_1)$$
$$+ \hat{I}_{2x} \sin(\Omega_2 t_1) \cos(\pi J_{12} t_1) - 2 \hat{I}_{1y} \hat{I}_{2z} \sin(\Omega_2 t_1) \sin(\pi J_{12} t_1)$$

**Conclusions:**

③  $\Omega_1$  at  $t_1$  &  $\Omega_2$  at  $t_2$



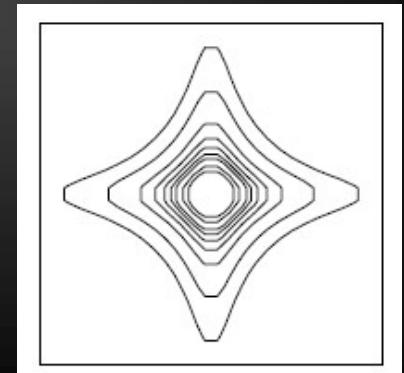
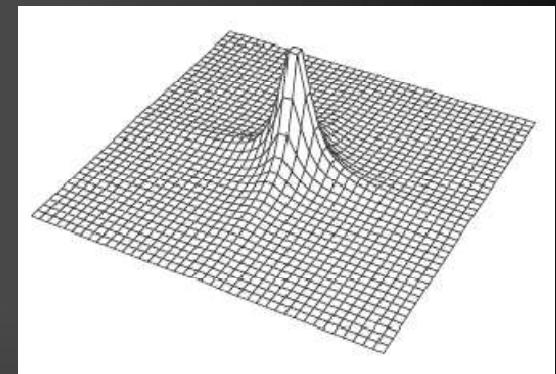
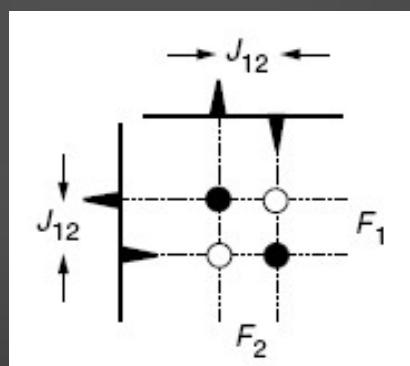
**Cross-peak**

$$- 2 \hat{I}_{1z} \hat{I}_{2y} \sin(\Omega_1 t_1) \sin(\pi J_{12} t_1)$$



$$\frac{1}{2} [-\cos(\Omega_1 t_1 + \pi J_{12} t_1) + \cos(\Omega_1 t_1 - \pi J_{12} t_1)]$$

**Doubly Absorptive**



# COSY

## Product operator formalism:

$$+ \hat{I}_{1x} \sin(\Omega_1 t_1) \cos(\pi J_{12} t_1) - 2 \hat{I}_{1z} \hat{I}_{2y} \sin(\Omega_1 t_1) \sin(\pi J_{12} t_1)$$

$$+ \hat{I}_{2x} \sin(\Omega_2 t_1) \cos(\pi J_{12} t_1) - 2 \hat{I}_{1y} \hat{I}_{2z} \sin(\Omega_2 t_1) \sin(\pi J_{12} t_1)$$

**4<sup>th</sup> stage (acquisition): *chemical shift* ( $\Omega$ ) and ( $J$ ) evolution at  $t_2$**

$$\xrightarrow{\Omega_1 t_2 \hat{I}_{1z} + \Omega_2 t_2 \hat{I}_{2z}}$$

$$+ \hat{I}_{1x} \sin(\Omega_1 t_1) \cos(\pi J_{12} t_1) \cos(\Omega_1 t_2) + \hat{I}_{1y} \sin(\Omega_1 t_1) \cos(\pi J_{12} t_1) \sin(\Omega_1 t_2)$$

$$- 2 \hat{I}_{1z} \hat{I}_{2y} \sin(\Omega_1 t_1) \sin(\pi J_{12} t_1) \cos(\Omega_2 t_2) + 2 \hat{I}_{1z} \hat{I}_{2x} \sin(\Omega_1 t_1) \sin(\pi J_{12} t_1) \sin(\Omega_2 t_2)$$

$$+ \hat{I}_{2x} \sin(\Omega_2 t_1) \cos(\pi J_{12} t_1) \cos(\Omega_2 t_2) + \hat{I}_{2y} \sin(\Omega_2 t_1) \cos(\pi J_{12} t_1) \sin(\Omega_2 t_2)$$

$$- 2 \hat{I}_{1y} \hat{I}_{2z} \sin(\Omega_2 t_1) \sin(\pi J_{12} t_1) \cos(\Omega_1 t_2) + 2 \hat{I}_{1x} \hat{I}_{2z} \sin(\Omega_2 t_1) \sin(\pi J_{12} t_1) \sin(\Omega_1 t_2)$$

$$\xrightarrow{\pi J_{12} t_2 2(\hat{I}_{1z} \hat{I}_{2z})}$$

**COSY**

## Product operator formalism:

$$\begin{aligned} & + \hat{I}_{1x} \sin(\Omega_1 t_1) \cos(\pi J_{12} t_1) \cos(\Omega_1 t_2) \cos(\pi J_{12} t_2) + 2 \hat{I}_{1y} \hat{I}_{2z} \sin(\Omega_1 t_1) \cos(\pi J_{12} t_1) \cos(\Omega_1 t_2) \sin(\pi J_{12} t_2) \\ & + \hat{I}_{1y} \sin(\Omega_1 t_1) \cos(\pi J_{12} t_1) \sin(\Omega_1 t_2) \cos(\pi J_{12} t_2) - 2 \hat{I}_{1x} \hat{I}_{2z} \sin(\Omega_1 t_1) \cos(\pi J_{12} t_1) \sin(\Omega_1 t_2) \sin(\pi J_{12} t_2) \\ & - 2 \hat{I}_{1z} \hat{I}_{2y} \sin(\Omega_1 t_1) \sin(\pi J_{12} t_1) \cos(\Omega_2 t_2) \cos(\pi J_{12} t_2) + \hat{I}_{2x} \sin(\Omega_1 t_1) \sin(\pi J_{12} t_1) \cos(\Omega_2 t_2) \sin(\pi J_{12} t_2) \\ & - 2 \hat{I}_{1z} \hat{I}_{2x} \sin(\Omega_1 t_1) \sin(\pi J_{12} t_1) \sin(\Omega_2 t_2) \cos(\pi J_{12} t_2) + \hat{I}_{2y} \sin(\Omega_1 t_1) \sin(\pi J_{12} t_1) \sin(\Omega_2 t_2) \sin(\pi J_{12} t_2) \\ & + \hat{I}_{2x} \sin(\Omega_2 t_1) \cos(\pi J_{12} t_1) \cos(\Omega_2 t_2) \cos(\pi J_{12} t_2) + 2 \hat{I}_{1z} \hat{I}_{2y} \sin(\Omega_2 t_1) \cos(\pi J_{12} t_1) \cos(\Omega_2 t_2) \sin(\pi J_{12} t_2) \\ & + \hat{I}_{2y} \sin(\Omega_2 t_1) \cos(\pi J_{12} t_1) \sin(\Omega_2 t_2) \cos(\pi J_{12} t_2) - 2 \hat{I}_{1z} \hat{I}_{2x} \sin(\Omega_2 t_1) \cos(\pi J_{12} t_1) \sin(\Omega_2 t_2) \sin(\pi J_{12} t_2) \\ & - 2 \hat{I}_{1y} \hat{I}_{2z} \sin(\Omega_2 t_1) \sin(\pi J_{12} t_1) \cos(\Omega_1 t_2) \cos(\pi J_{12} t_2) + \hat{I}_{1x} \sin(\Omega_2 t_1) \sin(\pi J_{12} t_1) \cos(\Omega_1 t_2) \sin(\pi J_{12} t_2) \\ & - 2 \hat{I}_{1x} \hat{I}_{2z} \sin(\Omega_2 t_1) \sin(\pi J_{12} t_1) \sin(\Omega_1 t_2) \cos(\pi J_{12} t_2) + \hat{I}_{1y} \sin(\Omega_2 t_1) \sin(\pi J_{12} t_1) \sin(\Omega_1 t_2) \sin(\pi J_{12} t_2) \end{aligned}$$

# COSY

## Product operator formalism:

$$\begin{aligned}
 & + \hat{I}_{1x} \sin(\Omega_1 t_1) \cos(\pi J_{12} t_1) \cos(\Omega_1 t_2) \cos(\pi J_{12} t_2) + 2 \hat{I}_{1y} \hat{I}_{2z} \sin(\Omega_1 t_1) \cos(\pi J_{12} t_1) \cos(\Omega_1 t_2) \sin(\pi J_{12} t_2) \\
 & + \hat{I}_{1y} \sin(\Omega_1 t_1) \cos(\pi J_{12} t_1) \sin(\Omega_1 t_2) \cos(\pi J_{12} t_2) - 2 \hat{I}_{1x} \hat{I}_{2z} \sin(\Omega_1 t_1) \cos(\pi J_{12} t_1) \sin(\Omega_1 t_2) \sin(\pi J_{12} t_2) \\
 & - 2 \hat{I}_{1z} \hat{I}_{2y} \sin(\Omega_1 t_1) \sin(\pi J_{12} t_1) \cos(\Omega_2 t_2) \cos(\pi J_{12} t_2) + \hat{I}_{2x} \sin(\Omega_1 t_1) \sin(\pi J_{12} t_1) \cos(\Omega_2 t_2) \sin(\pi J_{12} t_2) \\
 & - 2 \hat{I}_{1z} \hat{I}_{2x} \sin(\Omega_1 t_1) \sin(\pi J_{12} t_1) \sin(\Omega_2 t_2) \cos(\pi J_{12} t_2) + \hat{I}_{2y} \sin(\Omega_1 t_1) \sin(\pi J_{12} t_1) \sin(\Omega_2 t_2) \sin(\pi J_{12} t_2) \\
 & + \hat{I}_{2x} \sin(\Omega_2 t_1) \cos(\pi J_{12} t_1) \cos(\Omega_2 t_2) \cos(\pi J_{12} t_2) + 2 \hat{I}_{1z} \hat{I}_{2y} \sin(\Omega_2 t_1) \cos(\pi J_{12} t_1) \cos(\Omega_2 t_2) \sin(\pi J_{12} t_2) \\
 & + \hat{I}_{2y} \sin(\Omega_2 t_1) \cos(\pi J_{12} t_1) \sin(\Omega_2 t_2) \cos(\pi J_{12} t_2) - 2 \hat{I}_{1z} \hat{I}_{2x} \sin(\Omega_2 t_1) \cos(\pi J_{12} t_1) \sin(\Omega_2 t_2) \sin(\pi J_{12} t_2) \\
 & - 2 \hat{I}_{1y} \hat{I}_{2z} \sin(\Omega_2 t_1) \sin(\pi J_{12} t_1) \cos(\Omega_1 t_2) \cos(\pi J_{12} t_2) + \hat{I}_{1x} \sin(\Omega_2 t_1) \sin(\pi J_{12} t_1) \cos(\Omega_1 t_2) \sin(\pi J_{12} t_2) \\
 & - 2 \hat{I}_{1x} \hat{I}_{2z} \sin(\Omega_2 t_1) \sin(\pi J_{12} t_1) \sin(\Omega_1 t_2) \cos(\pi J_{12} t_2) + \hat{I}_{1y} \sin(\Omega_2 t_1) \sin(\pi J_{12} t_1) \sin(\Omega_1 t_2) \sin(\pi J_{12} t_2)
 \end{aligned}$$

