

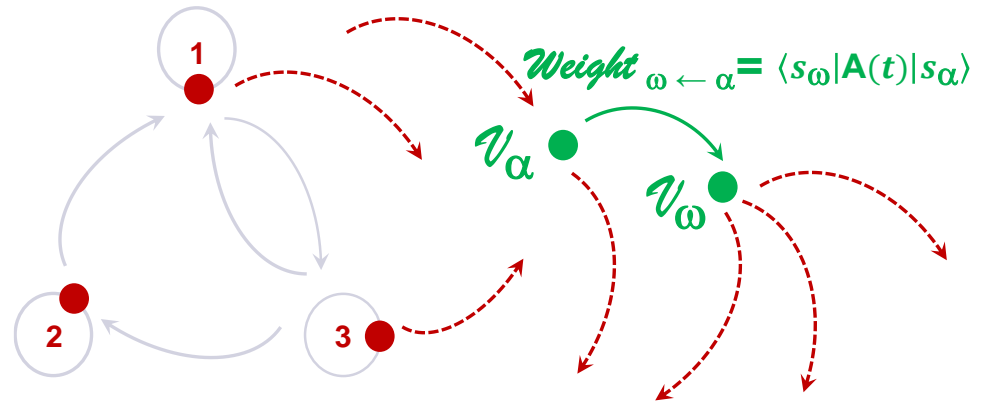
# Theory of Solid State NMR: from Dyson, Magnus, Feynman to *Path-Sum*

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## General context

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- consider the mathematical problem of coupled LDE with non-constant coefficients  $a(t')$ ,  $b(t')$ ...

$$A(t')U(t', t) = \frac{d}{dt'}U(t', t), \quad U(t, t) = \text{Id},$$

The diagram shows a matrix  $A(t')$  with elements  $a(t')$ ,  $b(t')$ ,  $c(t')$ , and ellipses. A yellow double-headed arrow above the matrix is labeled "N (finite)". To the right of the matrix is the letter "N". A yellow circle highlights the bottom-right ellipsis, with the text "bounded (over [ t , t' ])" next to it.

$$A(t') = \begin{pmatrix} a(t') & b(t') & \dots \\ c(t') & \dots & \dots \\ \dots & \dots & \dots \end{pmatrix} \quad \text{N}$$

bounded (over [ t , t' ])

— Dyson time-ordering operator (1952)

$$U(t', t) = \mathcal{T} \exp \left( \int_t^{t'} A(\tau) d\tau \right)$$

— Floquet (1883) (if  $A$  periodic)

Magnus (1954)



**perturbative treatment  
convergence (?)**

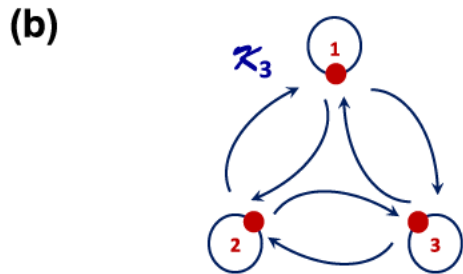
# The Path-Sum approach (P.-L. Giscard, 2015)

## ► Descending Ladder Principle (DLP)

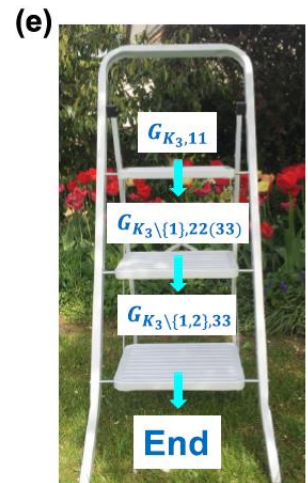
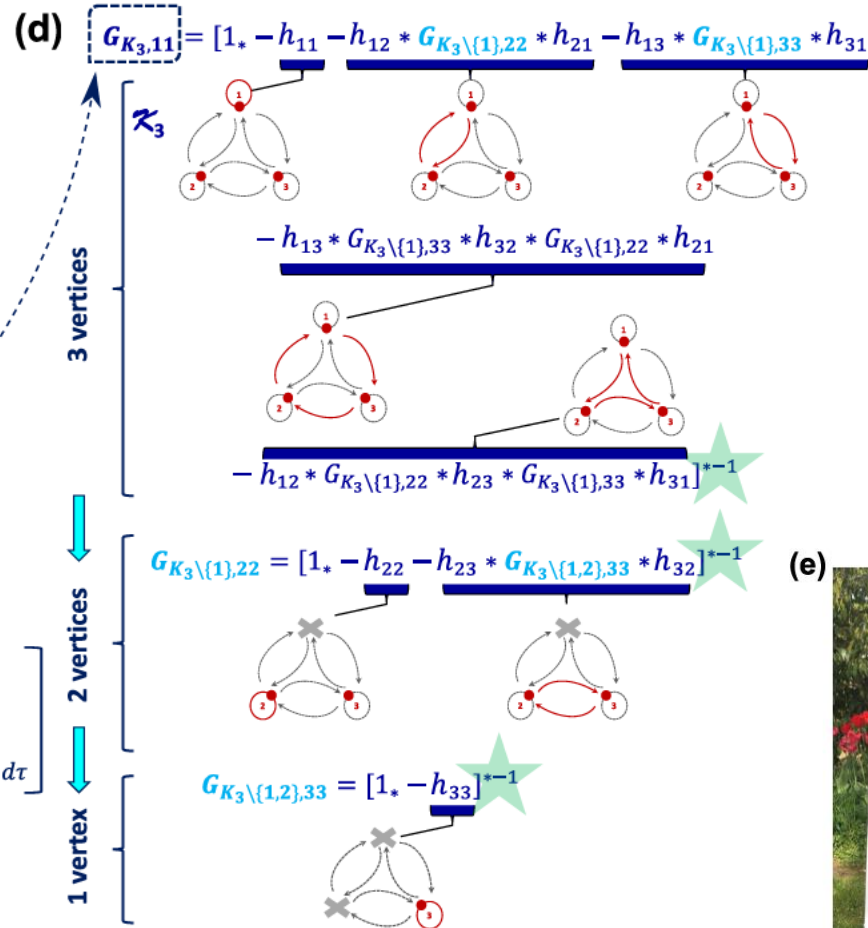
$$(f \star g) = \int_t^{t'} f(t', \tau) g(\tau, t) d\tau$$

$$[1_\star - (\star \star \star \dots)]^{\star-1} = \sum_{n \geq 0} (\star \star \star \dots)^{\star n}$$

(a) 
$$H(t) = \begin{pmatrix} h_{11}(t) & h_{12}(t) & h_{13}(t) \\ h_{21}(t) & h_{22}(t) & h_{23}(t) \\ h_{31}(t) & h_{32}(t) & h_{33}(t) \end{pmatrix}$$



(c) 
$$u(t', t) = \begin{bmatrix} \int_t^{t'} G_{K_3,11}(\tau, t) d\tau & U_{12}(t', t) & U_{13}(t', t) \\ U_{21}(t', t) & \int_t^{t'} G_{K_3,22}(\tau, t) d\tau & U_{23}(t', t) \\ U_{31}(t', t) & U_{32}(t', t) & \int_t^{t'} G_{K_3,33}(\tau, t) d\tau \end{bmatrix}$$



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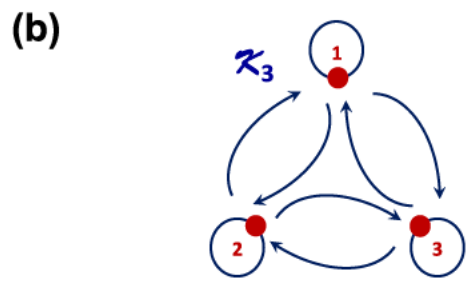
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dynamical weighted graph ( $\mathcal{G}$ )

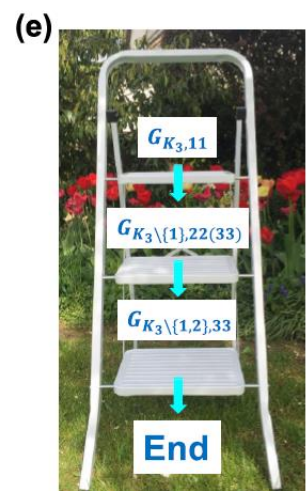
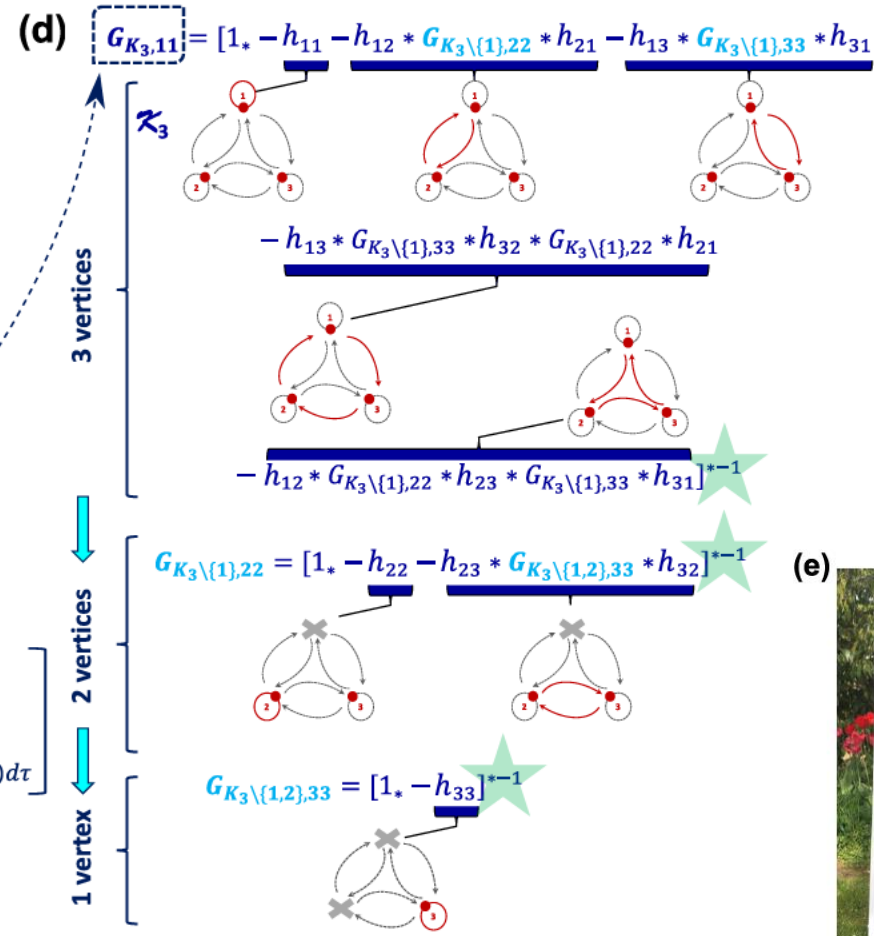
(a)

$$\begin{pmatrix} h_{12}(t) & h_{13}(t) \\ h_{21}(t) & h_{22}(t) & h_{23}(t) \\ h_{31}(t) & h_{32}(t) & h_{33}(t) \end{pmatrix}$$



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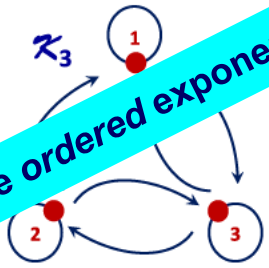
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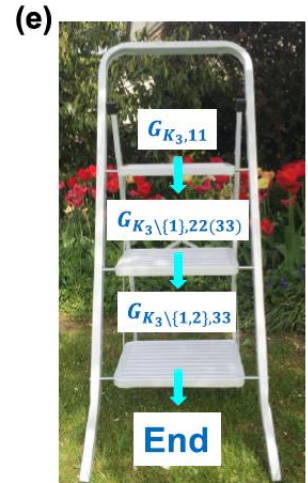
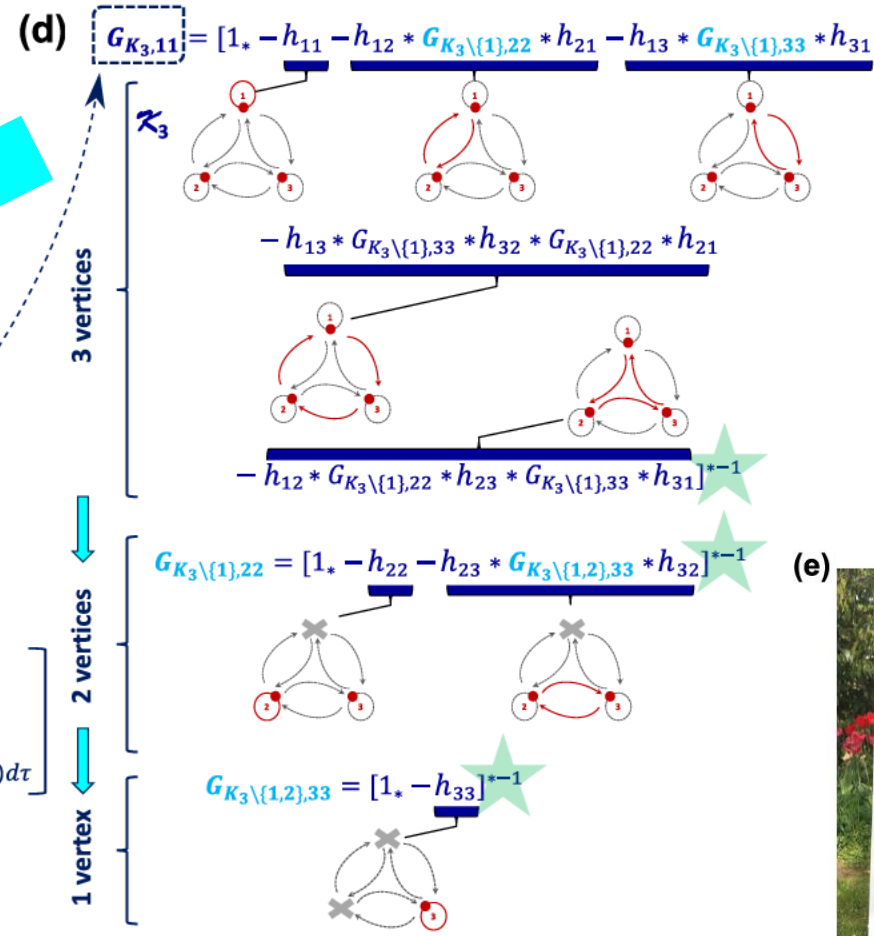
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 h_{12}(t) & h_{13}(t) \\
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 \end{pmatrix}$$

$U(t', t)$  as the ordered exponential of  $H(t)$



(c)

$$U(t', t) = \begin{bmatrix} \int_t^{t'} G_{K_3,11}(\tau, t) d\tau & U_{12}(t', t) & U_{13}(t', t) \\ U_{21}(t', t) & \int_t^{t'} G_{K_3,22}(\tau, t) d\tau & U_{23}(t', t) \\ U_{31}(t', t) & U_{32}(t', t) & \int_t^{t'} G_{K_3,33}(\tau, t) d\tau \end{bmatrix}$$



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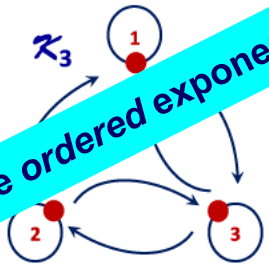
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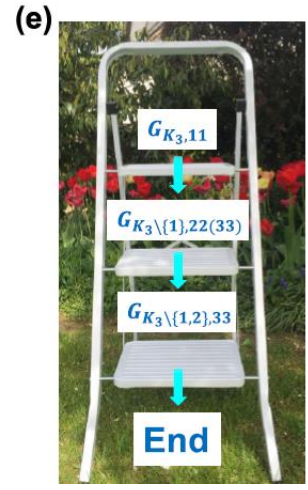
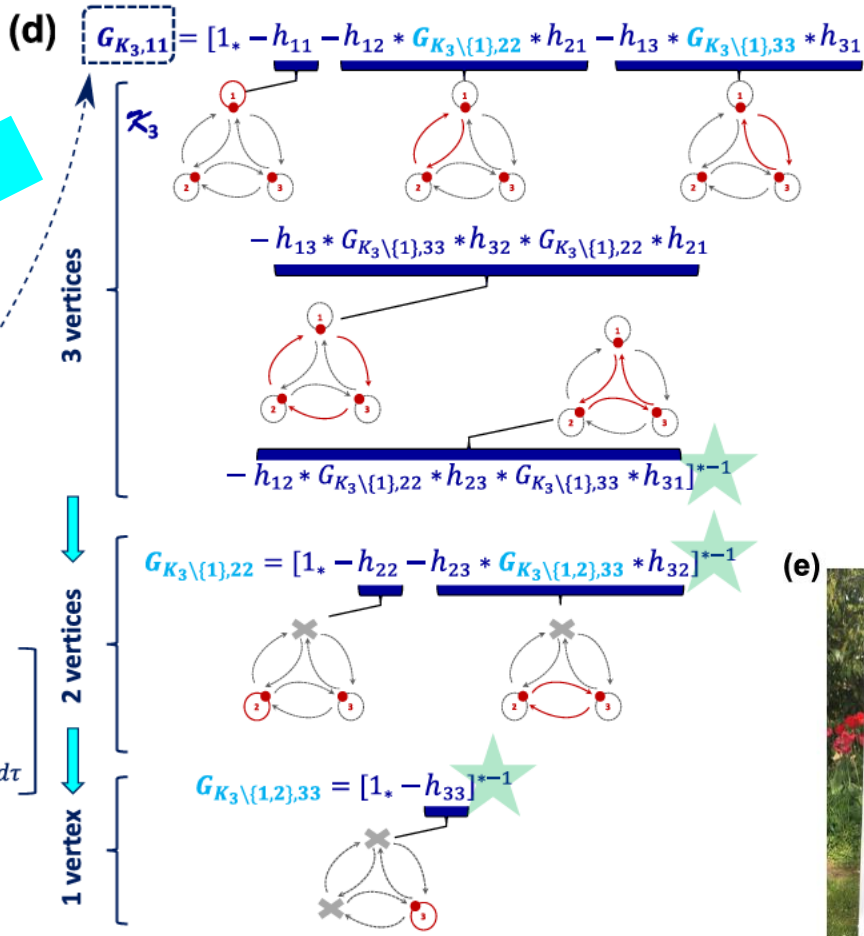
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(b)  $U(t', t)$  as the ordered exponential of  $H(t)$



(c) each entry is given analytically

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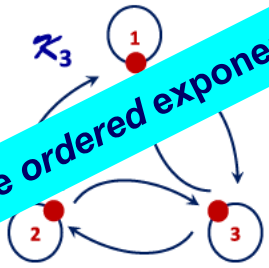
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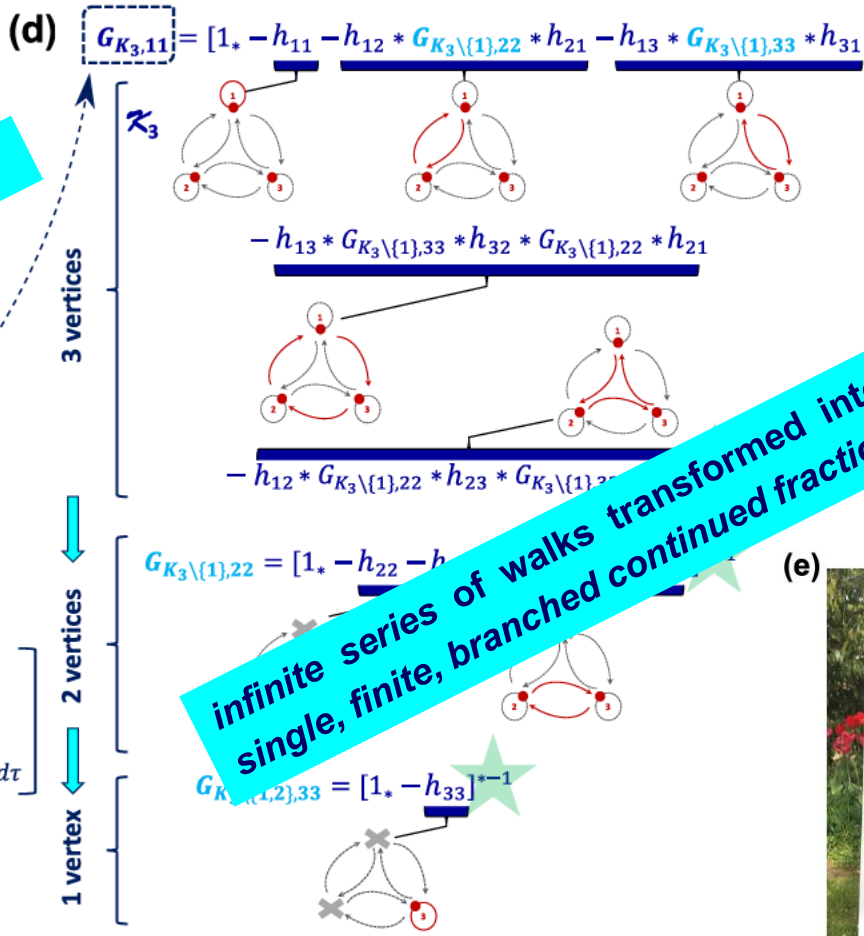
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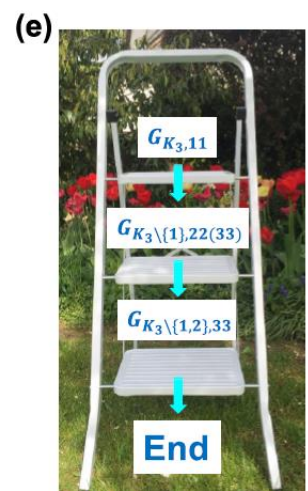


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infinite series of walks transformed into a single, finite, branched continued fraction



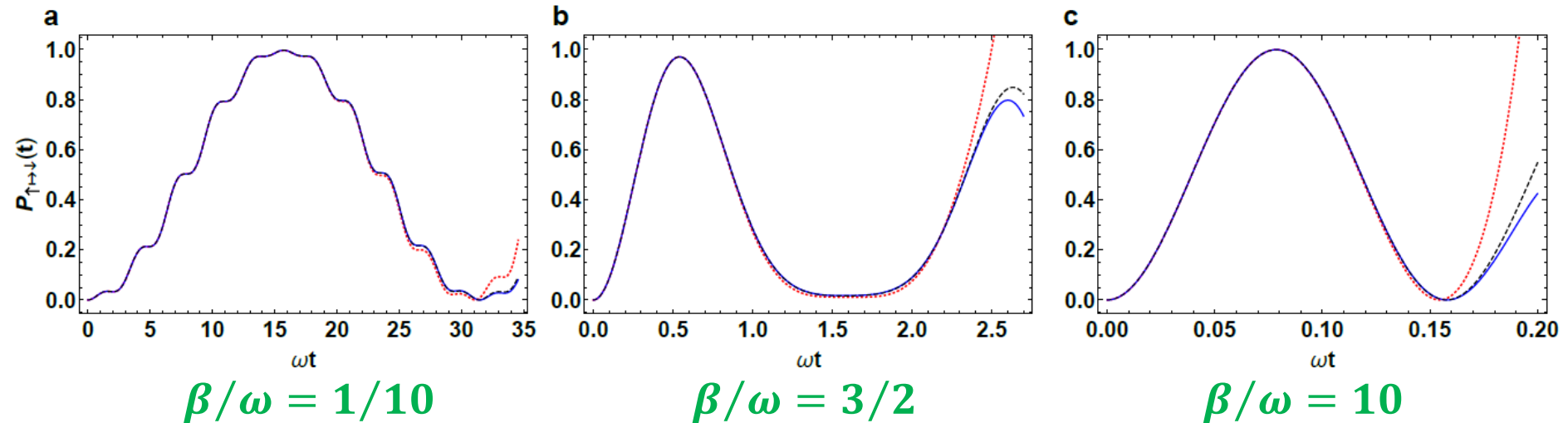
# A test example (NMR, qubit physics...)

$$\mathbf{H}(t) = \frac{1}{2} \omega_0 \boldsymbol{\sigma}_z + 2\beta \boldsymbol{\sigma}_x \cos(\omega t)$$

$$\mathbf{H}(t) = \begin{pmatrix} \frac{\omega_0}{2} & 2\beta \cos(\omega t) \\ 2\beta \cos(\omega t) & -\frac{\omega_0}{2} \end{pmatrix}$$

**P(t) transition probability**

**$\omega = \omega_0$  or  $\omega \neq \omega_0$**

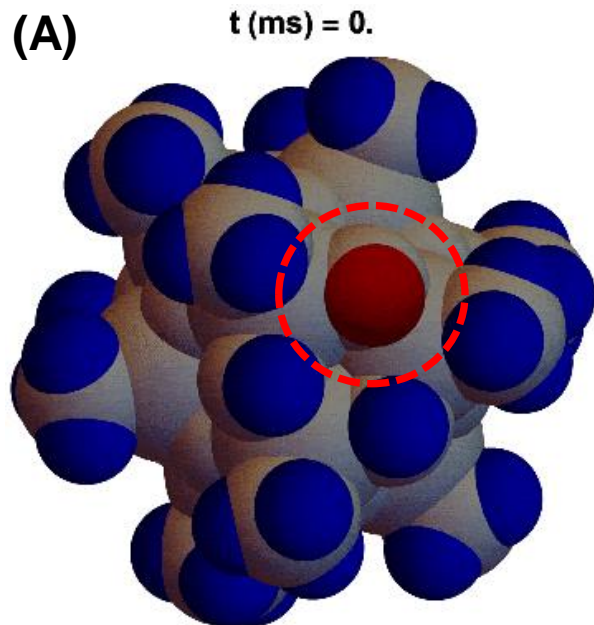


► Bloch-Siegert effect



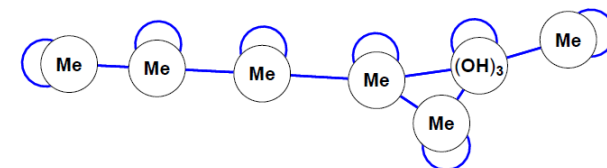
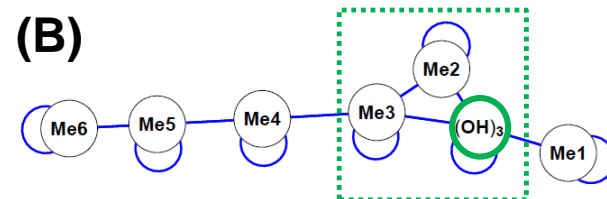
# Scale invariance of Path-Sum

► Path-Sum can be used in conjunction with all *state-space reduction* techniques



$(\text{CH}_3)_{12}(\text{OH})_6\text{Sn}_{12}$   
42 protons  
MAS 10 kHz  
pure state

**PARTITIONS**



(C)

$$U_{(\text{OH})_3} = 1 * \left( \text{Id}_* + iH_{(\text{OH})_3} + H_{(\text{OH})_3\text{Me}_1} * \Gamma_1 * H_{\text{Me}_1(\text{OH})_3} \right. \\ \left. + H_{(\text{OH})_3\text{Me}_2} * \Sigma_2 * H_{\text{Me}_2(\text{OH})_3} + H_{(\text{OH})_3\text{Me}_3} * \Sigma_3 * H_{\text{Me}_3(\text{OH})_3} \right. \\ \left. - i H_{(\text{OH})_3\text{Me}_2} * \Gamma_2 * H_{\text{Me}_2\text{Me}_3} * \Sigma_3 * H_{\text{Me}_3(\text{OH})_3} \right. \\ \left. - i H_{(\text{OH})_3\text{Me}_3} * \Sigma_3 * H_{\text{Me}_3\text{Me}_2} * \Sigma_2 * H_{\text{Me}_2(\text{OH})_3} \right)^{-1},$$

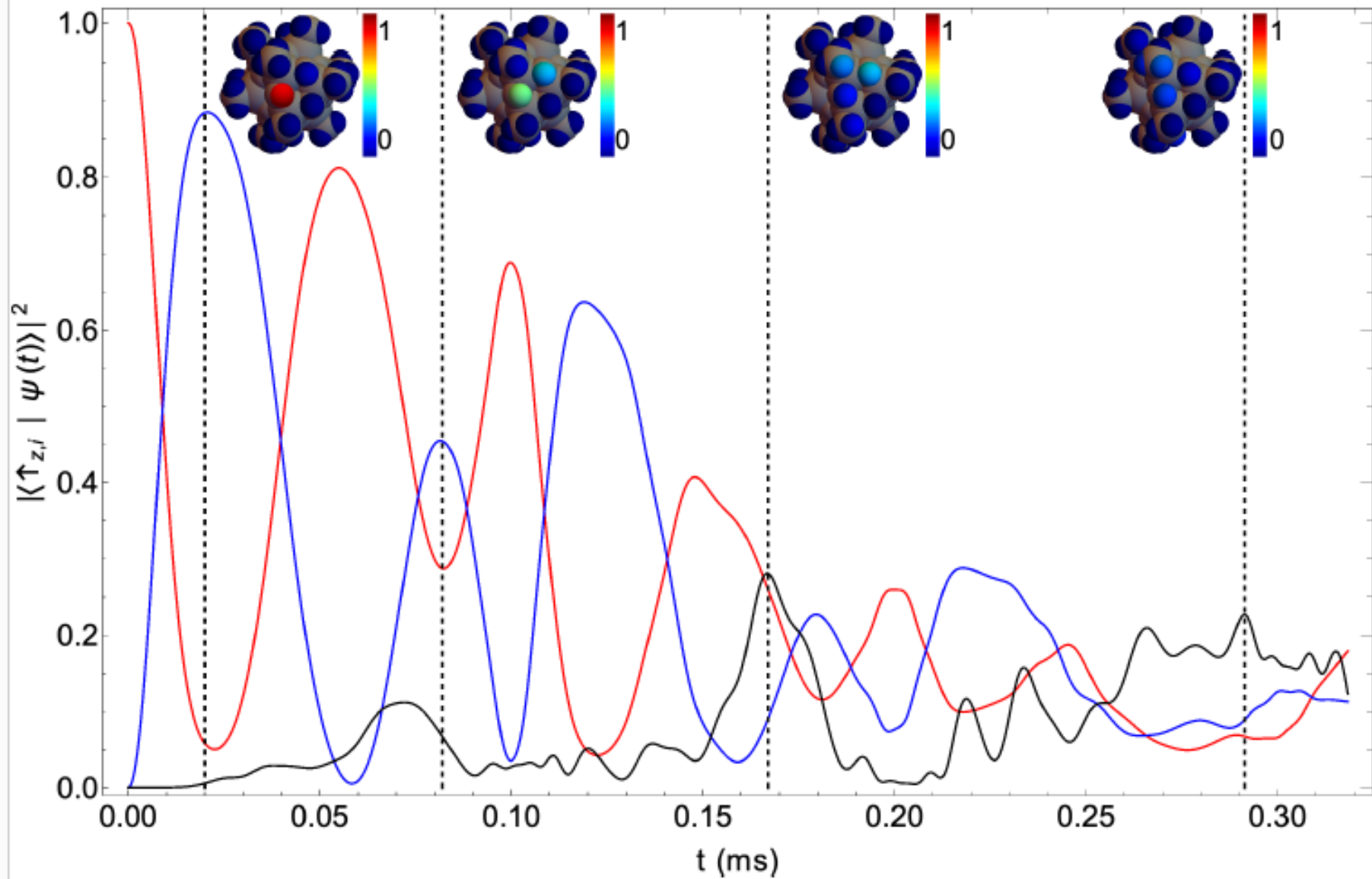
$$\Sigma_2 = \frac{1}{\text{Id}_* + iH_{\text{Me}_2} + H_{\text{Me}_2\text{Me}_3} * \Sigma_3 * H_{\text{Me}_3\text{Me}_2}},$$

$$\Sigma_3 = \frac{1}{\text{Id}_* + iH_{\text{Me}_3} + H_{\text{Me}_3\text{Me}_4} * \Sigma_4 * H_{\text{Me}_4\text{Me}_3}},$$

$$\Sigma_4 = \frac{1}{\text{Id}_* + iH_{\text{Me}_4} + H_{\text{Me}_4\text{Me}_5} * \Sigma_5 * H_{\text{Me}_5\text{Me}_4}},$$

$$\Sigma_5 = \frac{1}{\text{Id}_* + iH_{\text{Me}_5} + H_{\text{Me}_5\text{Me}_6} * \Gamma_6 * H_{\text{Me}_6\text{Me}_5}},$$

# Scale invariance of Path-Sum



### Path-Sum



- ▶ a new approach
- ▶ analytical expression for  $U(t)$
- ▶ unconditional convergence
- ▶ non perturbative formulation
- ▶ scalable to large spin systems
- ▶ other theory/applications to come...

(very) warm thanks to P.-L. Giscard

Ass. Pr. in Calais, France

Liouville laboratory

*Algebraic Combinatorials*

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