Path-Sum: a New Avenue for Spin Dynamics

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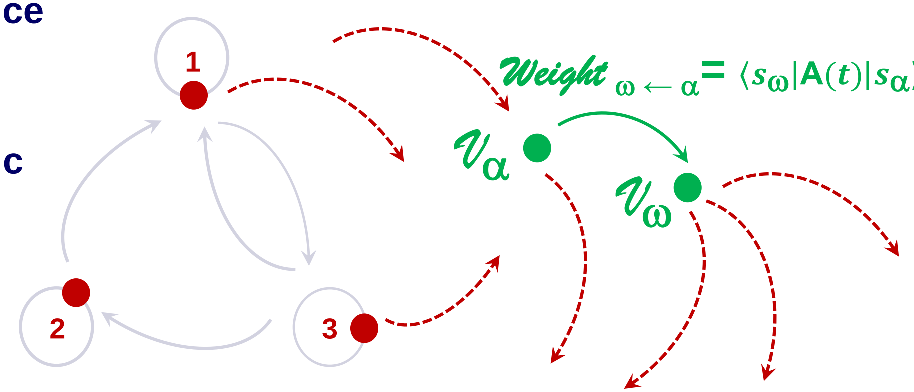

GDCh
Gesellschaft Deutscher Chemiker

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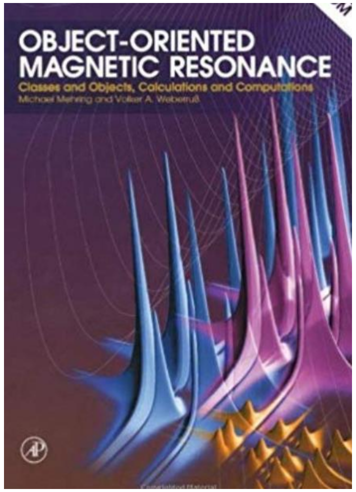
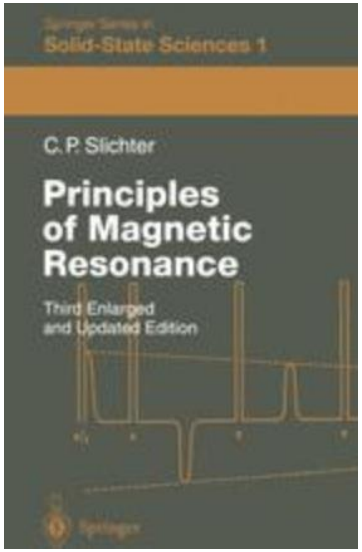
FGMR 2022

Standard equations in NMR





- **Schrödinger equation**

state vector

$$\frac{\partial}{\partial t}\,|\Psi(t)> = -\frac{i}{\hbar}\,\hat{H}(t)\,|\Psi(t)>$$

- **Liouville – von Neumann equation**

density operator

$$\frac{d}{dt}\,\hat{\rho}(t) = -\frac{i}{\hbar}\,[\hat{H}(t),\hat{\rho}(t)]$$

Dyson time-ordering operator

$$\hat{U}(\mathrm{t}',\mathrm{t}) = \mathrm{OE}\left[-\mathrm{i}\hat{U}(\mathrm{t}',\mathrm{t})\right] = \hat{T}\,\exp\left(-\mathrm{i}\int_t^{t'}\hat{U}(\tau)\mathrm{d}\tau\right)$$

→ evolution operator

→ « exponential » of a (time dependent) matrix

The evolution operator U(t)

► a general *mathematical* problem: coupled LDE with *non-constant* coefficients $a_{11}(t')$, $a_{12}(t')$…

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

N (finite)

$$\mathsf{A}(t') = \begin{pmatrix} a_{11}(t') & a_{12}(t') & \cdots \\ a_{21}(t') & a_{22}(t') & \cdots \\ \cdots & \cdots & \cdots \end{pmatrix} \; \mathsf{N}$$

bounded (over [*t* , *t’*])

The evolution operator U(t) and the ordered exponential

Dyson time-ordering operator

$$\hat{U}(t',t) = \mathrm{OE}\left[-i\hat{U}(t',t)\right] = \hat{T}\,\exp\left(-i\int_t^{t'}\hat{U}(\tau)\,d\tau\right)$$

Magnus **Floquet**

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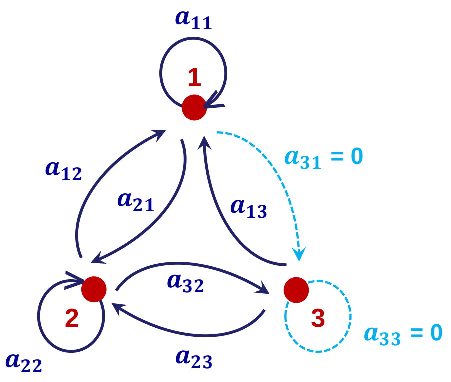
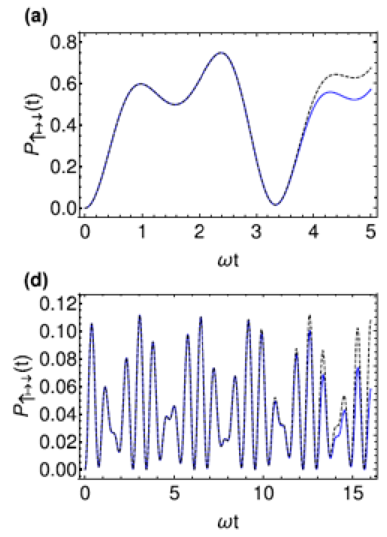
perturbative methods, convergence (?)

Outline

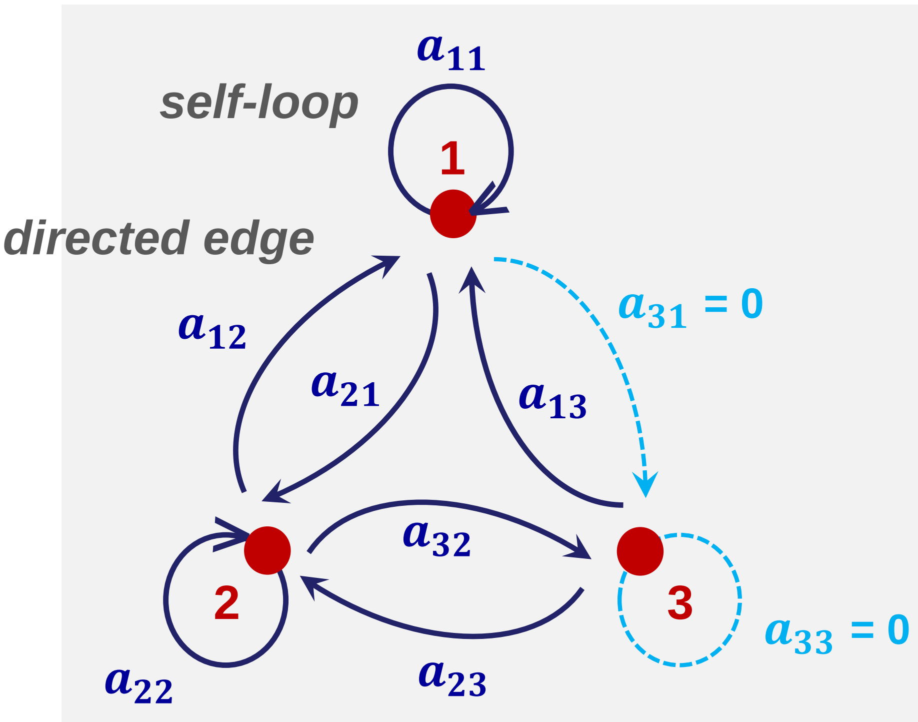
- Introduction to Path-Sum
- From Exponential to Ordered Exponential
- Analytical results
- Implementation in Mathematica





$\mathcal{G}$ = ($\mathcal{V}$ertex set, $\mathcal{E}$dge set)

Adjacency *finite* matrix $\mathbf{A}_{\mathcal{G}}$

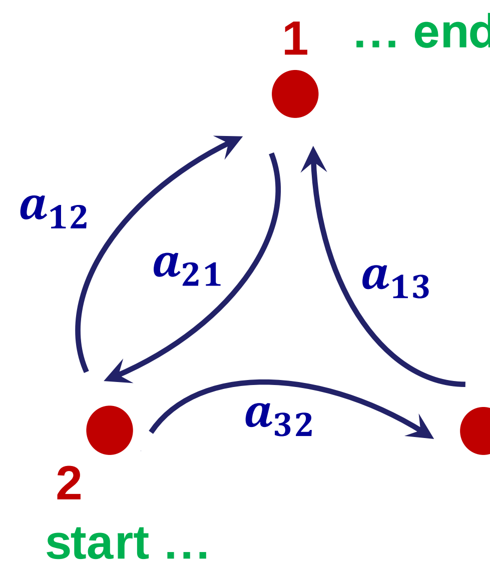


$$\mathbf{A}_{\mathcal{G}} = \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ 0 & a_{32} & 0 \end{pmatrix}$$

⬇

entry: *weight* on a ***directed edge***

ex.: ***walk*** $\mathcal{W}_{1\leftarrow 2}$ (from $\mathcal{V}_2$ **to** $\mathcal{V}_1$) of ***length* 4**



Giscard, 2012

An introduction to Path-Sum

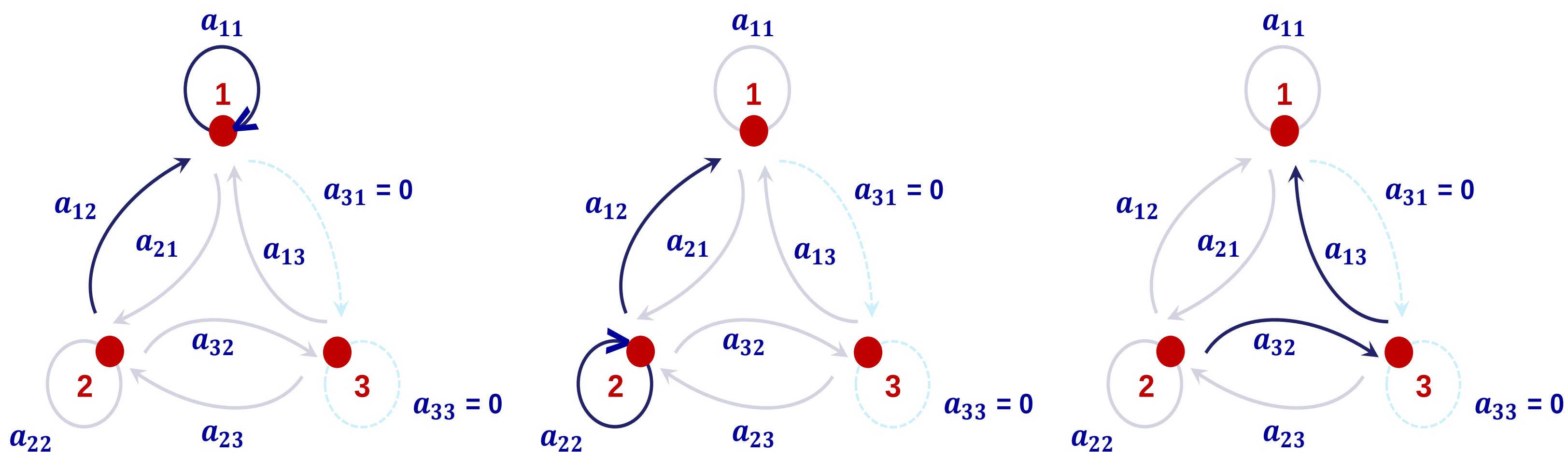
the *powers* of the Adjacency matrix $\mathbf{A}_{\mathcal{G}}$ on a graph $\mathcal{G}$ generate ALL *weighted* WALKS $\mathcal{W}$ on $\mathcal{G}$

$$a_{11} \times a_{12} + a_{12} \times a_{22} + a_{13} \times a_{32}$$

$$\mathbf{A}_{\mathcal{G}}^{2} = \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ 0 & a_{32} & 0 \end{pmatrix}^{2} = \begin{pmatrix} & \blacksquare & \\ \vdots & \ddots & \vdots \\ & \cdots & \end{pmatrix}$$

weighted $\mathcal{W}$ of ***length* 2** from v_2 to v_1

(1 ← 2)



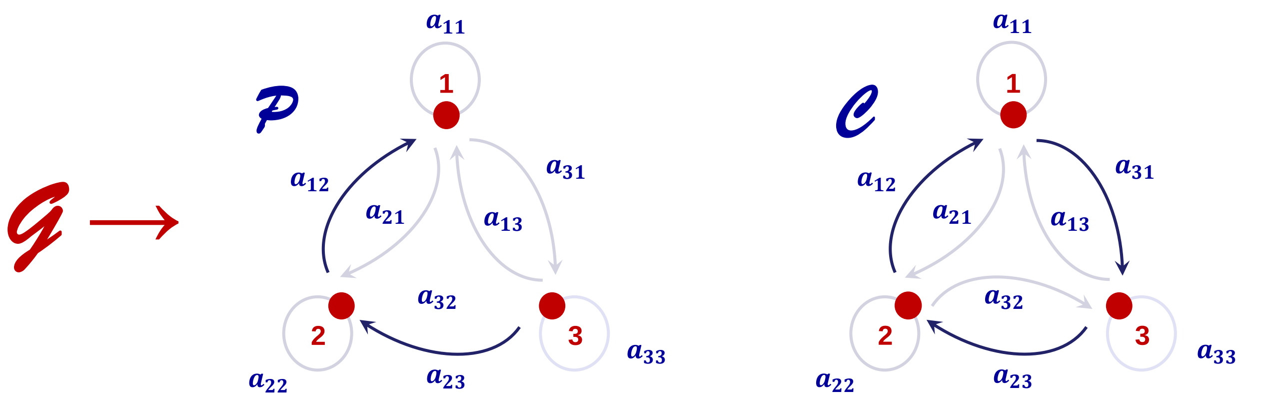
$$\Sigma = a_{11}a_{12} + a_{12}a_{22} + a_{13}a_{32}$$

N. Biggs: *Algebraic Graph Theory* (1993) **– *time-independent* matrices**

Simple paths and simple cycles

◊ ***simple path*** $\mathcal{P}$ (self avoiding walk): $\mathcal{W}$ whose $\mathcal{V}$ are all **distinct**

◊ ***simple cycle*** $\mathcal{C}$ (self avoiding polygon): $\mathcal{W}$ whose **endpoints** are **identical** and **intermediate** $\mathcal{V}$ are all **distinct** and different from the endpoints



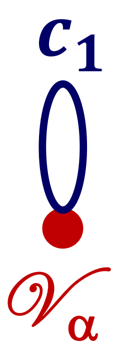
« Fundamental Theorem of Arithmetic on $\mathcal{G}$ » (Giscard, 2012)

► $\mathcal{W}$ factor ***uniquely*** into ***prime*** elements, *i.e.* ***simple paths*** and ***simple cycles***

► if $\mathcal{G}$ is ***finite*** the number of primes is ***finite***

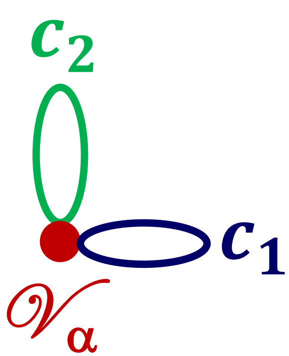
► resummation of all $\mathcal{W}$ involves a ***finite*** number of operations: ***sum*** *on* ***simple paths*** and ***continuous fraction*** *of* ***simple cycles*** with vertex removal

Resummation of $\mathscr{W}$ on a graph: an illustration



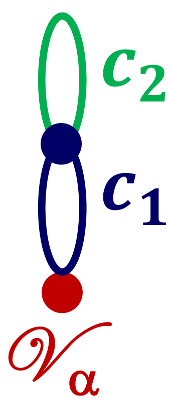
$$c_1 + c_1^2 + c_1^3 \ldots = \frac{1}{1 - c_1}$$

(fraction)



$$c_1 + c_1^2 + c_2 + c_1 c_2 c_1 \ldots = \frac{1}{1 - c_1 - c_2}$$

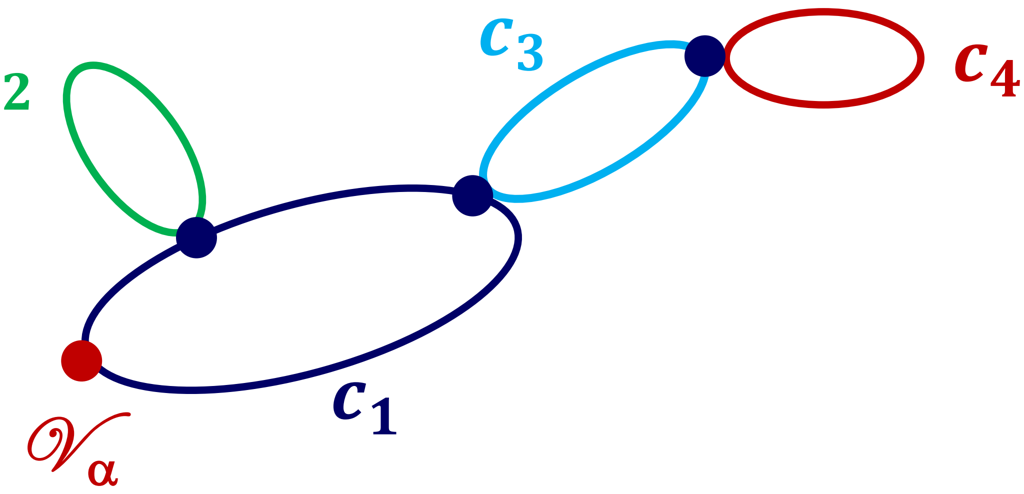
(fraction)



$$c_1 + c_1^2 + c_1 c_2 + \cdots = \frac{1}{1 - \frac{1}{1 - c_2} c_1}$$

(continued fraction)

Resummation of $\mathscr{W}$ on a graph: an illustration



$$\sum_{\mathscr{G}} (\mathscr{W}, c_i) = \frac{1}{1 - \frac{1}{1 - \frac{c_3}{1 - c_4}} \frac{1}{1 - c_2} c_1}$$

(continued fraction)

if $\mathscr{G}$ is *finite*: the continued fraction is *unique* and *finite*

Power series of $A_{\mathcal{G}}$

remember:

each element of $A_{\mathcal{G}}^{k}$ is given by the

sum of the *weighted* $\mathcal{W}$ of length k (standard × operation)

$$(A_{\mathcal{G}})^{k} = \begin{pmatrix} & \cdots & \\ \vdots & (A_{\mathcal{G}})^{k}_{\omega\alpha} & \vdots \\ & \cdots & \end{pmatrix}$$

$$F(A_{\mathcal{G}})_{\omega\alpha} = \sum_{k=0}^{\infty} c_k \sum_{\mathcal{W}_{\mathcal{G},\,\alpha\omega;\,k}} a_{\omega h_k} \cdots \times a_{h_3 h_2} \times a_{h_2 \alpha}$$

power series of $A_{\mathcal{G}}$

all *weighted* walks $\mathcal{W}$ **from** $\mathcal{V}_{\alpha}$ to $\mathcal{V}_{\omega}$ of length k

Power series of $A_{\mathcal{G}}$

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power series of $A_{\mathcal{G}}$ — all *weighted* walks $\mathcal{W}$ **from** $\mathcal{V}_\alpha$ to $\mathcal{V}_\omega$ of length k

Path-Sum

« Fundamental Theorem of Arithmetic » on $\mathcal{G}$ (Giscard, 2012)

► w factor ***uniquely*** into ***prime*** elements, *i.e*. ***simple paths*** and ***simple cycles***

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$$F(\mathrm{A}_{\mathcal{G}})_{\omega\alpha} = \sum_{k=0}^{\infty} c_k \sum_{\mathcal{W}_{\mathcal{G},\,\alpha\omega;\,k}} a_{\omega h_k} \cdots \times a_{h_3 h_2} \times a_{h_2 \alpha}$$

power series of $\mathbf{A}_{\mathcal{G}}$

all *weighted* walks $\mathcal{W}$ **from** $\mathcal{V}_{\alpha}$ to $\mathcal{V}_{\omega}$ of length k

Path-Sum

$$F(\mathrm{A}_{\mathcal{G}})_{\omega\alpha} = \sum_{\mathcal{P}_{\mathcal{G},\,\alpha\omega;\,\ell}} f(a_{\omega\omega}) \times a_{\omega\mu_{\ell}} \cdots f(a_{\mu_2\mu_2}) a_{\mu_2\alpha} \times f(a_{\alpha\alpha})$$

edge weight

effective $\mathcal{V}$ weight

sum on the ***finite*** set of

simple paths $\mathcal{P}$ of **length** ℓ

sum over the ***finite*** set of ***simple cycles*** $\mathcal{C}$

(***continued fraction*** of ***finite*** ***breadth***)

Giscard, *SIAM*, 2013

ex.: matrix EXPONENTIAL

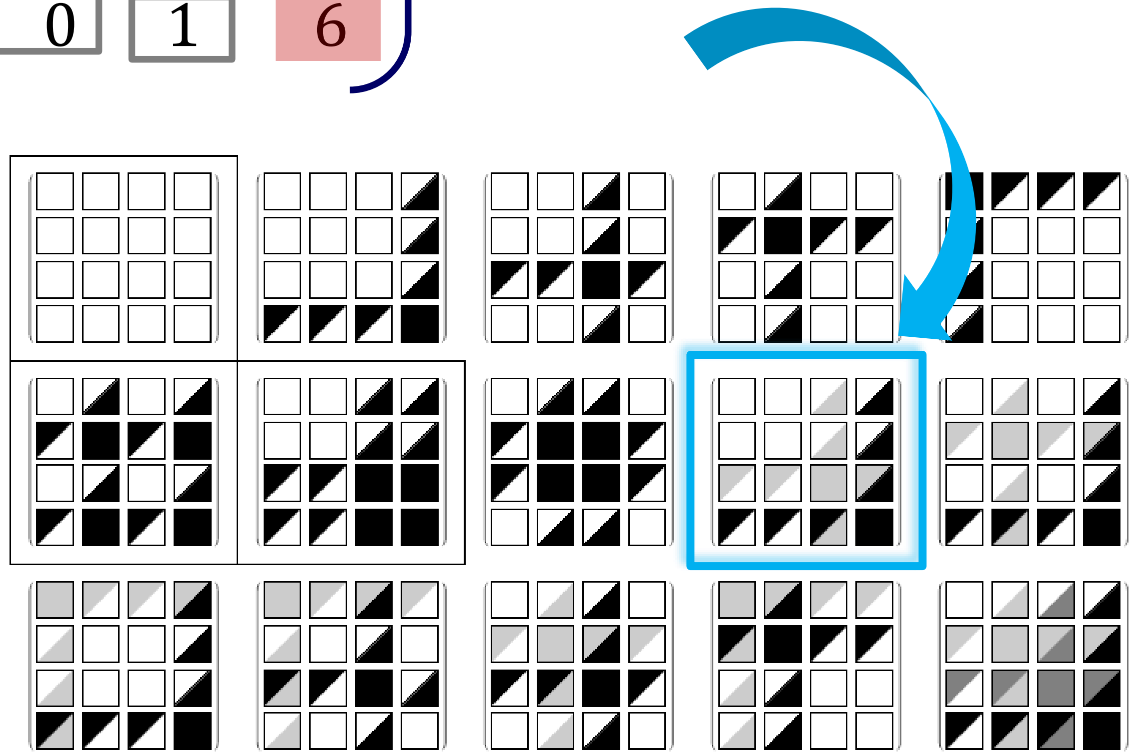
$$A = \begin{pmatrix} 1 & 2 & 1 & 0 \\ 3 & 4 & -8 & 0 \\ -5 & 9 & \boxed{5} & -3 \\ 0 & 0 & 1 & 6 \end{pmatrix}$$

entries: real, complex numbers, matrices, blocks of matrices….

$$e^{A} = \begin{pmatrix} 10.37 & 19.31 & -4.78 & 51.95 \\ 43.38 & -4.49 & -42.81 & 154.68 \\ -4.92 & 44.55 & \boxed{-25.70} & -35.24 \\ 18.96 & 49.55 & 11.74 & 363.50 \end{pmatrix}$$

Some operations on matrices $A_{\mathcal{G}}$ using Path-Sum

$$A = \begin{pmatrix} 1 & 2 & 1 & 0 \\ 3 & 4 & -8 & 0 \\ -5 & 9 & 5 & -3 \\ 0 & 0 & 1 & 6 \end{pmatrix}$$



one *partition* of A (among $B_4 = 15$)

Some operations on matrices $A_{\mathcal{G}}$ using Path-Sum

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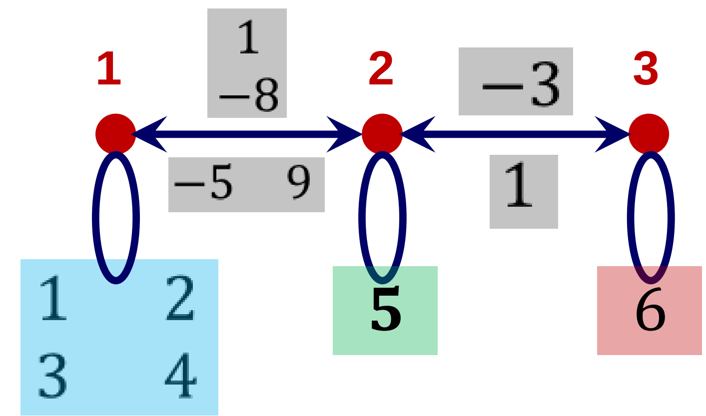

$\mathscr{P}$ath 3

$$\boxed{} = \mathscr{L}_{1(s,1)} \frac{1}{s - 5 - (-3)\frac{1}{s-6}(1) - (-5 \;\; 9)\left(\frac{1}{\begin{pmatrix} s-1 & -2 \\ -3 & s-4 \end{pmatrix}}\right)\begin{pmatrix} 1 \\ -8 \end{pmatrix}}$$

self-loop 2

self-loop 3

self-loop 1

$2 \rightarrow 3 \rightarrow 2$

$2 \rightarrow 1 \rightarrow 2$

Descending Ladder Principle (DLP)

$$e^A = \begin{pmatrix} \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \boxed{-25.70} & \cdots \\ \cdots & \cdots & \cdots & \cdots \end{pmatrix}$$

3 simple cycles ($\mathscr{C}$) from $\mathscr{V}_2 \rightarrow \mathscr{V}_2$

Some operations on matrices $A_{\mathcal{G}}$ using Path-Sum

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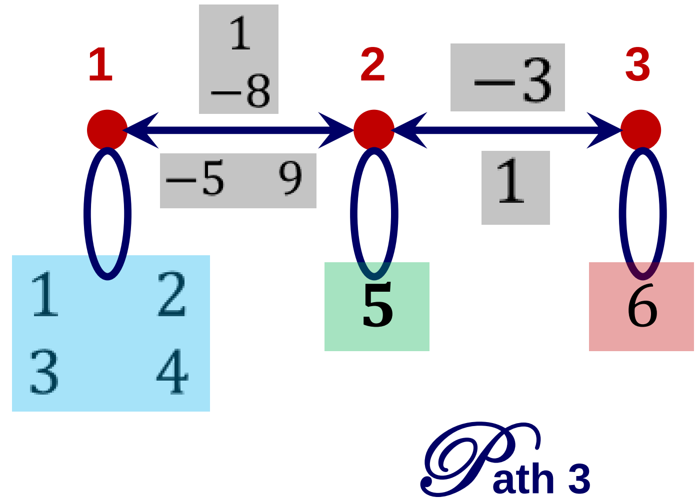

$$\boxed{} = \mathscr{L}^{-1}_{(s,1)} \frac{1}{s - 5 - (-3)\frac{1}{s-6}(1) - (-5\ \ 9)\left(\frac{1}{\begin{pmatrix} s-1 & -2 \\ -3 & s-4 \end{pmatrix}}\right)\begin{pmatrix} 1 \\ -8 \end{pmatrix}}$$

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3 simple cycles ($\mathscr{C}$) from $\mathscr{V}_2 \rightarrow \mathscr{V}_2$

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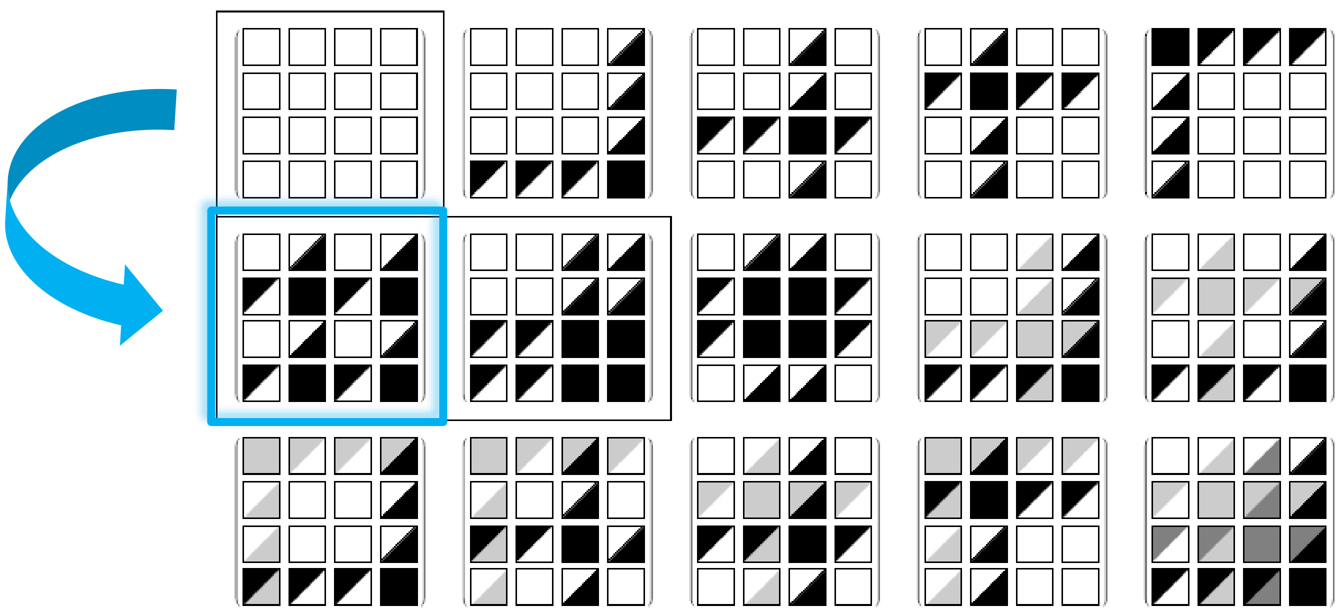
Some operations on matrices $A_{\mathcal{G}}$ using Path-Sum

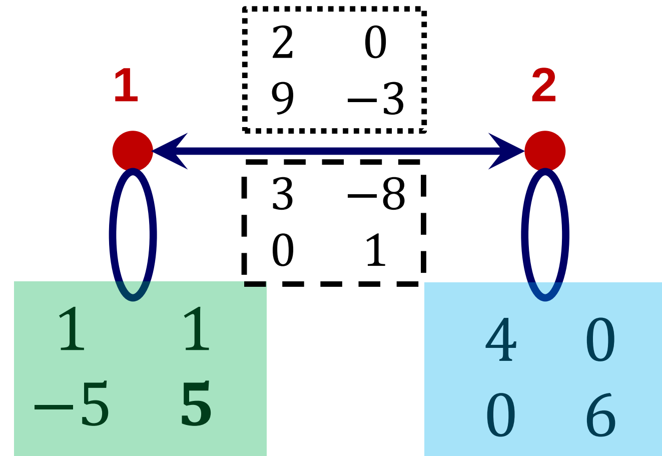
$$A = \begin{pmatrix} 1 & 2 & 1 & 0 \\ 3 & 4 & -8 & 0 \\ -5 & 9 & \mathbf{5} & -3 \\ 0 & 0 & 1 & 6 \end{pmatrix}$$



another *partition* of A (among $B_4 = 15$)

Some operations on matrices $A_{\mathcal{G}}$ using Path-Sum

$$A = \begin{pmatrix} 1 & 2 & 1 & 0 \\ 3 & 4 & -8 & 0 \\ -5 & 9 & 5 & -3 \\ 0 & 0 & 1 & 6 \end{pmatrix}$$



$$\mathscr{L}_{1(s,1)} = \frac{1}{\begin{pmatrix} s & 0 \\ 0 & s \end{pmatrix} - \begin{pmatrix} 1 & 1 \\ -5 & 5 \end{pmatrix} - \begin{pmatrix} 2 & 0 \\ 9 & -3 \end{pmatrix} \left(\frac{1}{\begin{pmatrix} s-4 & 0 \\ 0 & s-6 \end{pmatrix}} \right) \begin{pmatrix} 3 & -8 \\ 0 & 1 \end{pmatrix}}$$

self-loop 1

self-loop 2

$1 \to 2 \to 1$

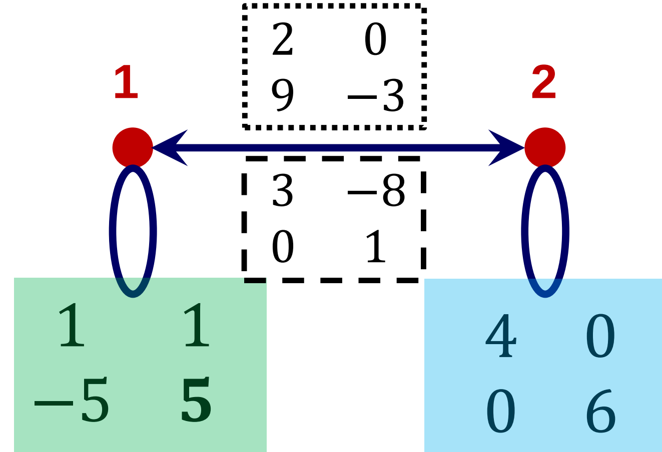
$\mathscr{K}_2$

$$e^A = \begin{pmatrix} 10.37 & \dots & -4.78 & \dots \\ \dots & \dots & \dots & \dots \\ -4.92 & \dots & \boxed{\mathbf{-25.70}} & \dots \\ \dots & \dots & \dots & \dots \end{pmatrix}$$

2 simple cycles ($\mathscr{C}$) from $\mathscr{V}_1 \to \mathscr{V}_1$

Some operations on matrices $A_{\mathcal{G}}$ using Path-Sum

$$e^{A} = \begin{pmatrix} 10.37 & 19.31 & -4.78 & 51.95 \\ 43.38 & -4.49 & -42.81 & 154.68 \\ -4.92 & 44.55 & -25.70 & -35.24 \\ 18.96 & 49.55 & 11.74 & 363.50 \end{pmatrix}$$



$\mathcal{K}_2$

$$\mathcal{L}_{1(s,1)} = \frac{1}{\begin{pmatrix} s & 0 \\ 0 & s \end{pmatrix} - \begin{pmatrix} 1 & 1 \\ -5 & 5 \end{pmatrix} - \begin{pmatrix} 2 & 0 \\ 9 & -3 \end{pmatrix} \left(\frac{1}{\begin{pmatrix} s-4 & 0 \\ 0 & s-6 \end{pmatrix}} \right) \begin{pmatrix} 3 & -8 \\ 0 & 1 \end{pmatrix}}$$

self-loop 1

self-loop 2

$1 \to 2 \to 1$

$$e^{A} = \begin{pmatrix} 10.37 & \dots & -4.78 & \dots \\ \dots & \dots & \dots & \dots \\ -4.92 & \dots & -25.70 & \dots \\ \dots & \dots & \dots & \dots \end{pmatrix}$$

2 simple cycles ($\mathcal{C}$) from $\mathcal{V}_1 \to \mathcal{V}_1$

Some operations on matrices $A_{\mathcal{G}}$ using Path-Sum

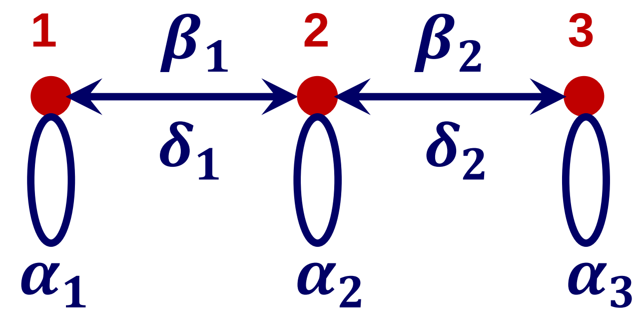
ex.: matrix INVERSE

Available online at www.sciencedirect.com
ScienceDirect
Applied Mathematics and Computation 197 (2008) 345–357
ELSEVIER
APPLIED MATHEMATICS AND COMPUTATION
www.elsevier.com/locate/amc

Explicit formula for the inverse of a tridiagonal matrix by backward continued fractions

Emrah Kılıç
TOBB University of Economics and Technology, Mathematics Department, 06560 Ankara, Turkey

2008



$\mathscr{P}$ath 3

$$T = [t_{ij}] = \begin{bmatrix} \alpha_1 & \beta_1 & 0 \\ \delta_1 & \alpha_2 & \beta_2 \\ 0 & \delta_2 & \alpha_3 \end{bmatrix}$$

$$t_{11}^{-1} = \frac{1}{C_1^b} + \frac{\beta_1\delta_1}{C_2^b (C_1^b)^2} + \frac{\beta_1\delta_1\beta_2\delta_2}{(C_1^b)^2 (C_2^b)^2 C_3^b}$$

$$= -\frac{\alpha_2\alpha_3 - \beta_2\delta_2}{\alpha_1\beta_2\delta_2 - \alpha_1\alpha_2\alpha_3 + \beta_1\alpha_3\delta_1},$$

$$\square = \cfrac{1}{\propto_1 - \beta_1 \cfrac{1}{\alpha_2 - \beta_2 \frac{1}{\alpha_3} \delta_2} \delta_1}$$

self-loop 1

self-loop 2

self-loop 3

$2 \rightarrow 3 \rightarrow 2$

$1 \rightarrow 2 \rightarrow 1$

easy to handle Path-Sum for $\mathscr{P}$ath (tridiagonal matrices)

Summary (partial)

- ► a **finite** *time-independent* matrix $\mathbf{A}_{\mathcal{G}}$ associated to $\mathcal{G}$ (bounded entries)

- ► each entry of a power series of $\mathbf{A}_{\mathcal{G}}$ is given by a **finite** number of operations by using Path-Sum (with $\times$ product)

- the matrix nature of the problem is fully replaced when working on entries

- or, one can keep it partially → **PARTITIONS** (**scalability**)

- calculations of **resolvents** by Path-Sum lead to **CLOSED-form** expressions when $\mathbf{A}_{\mathcal{G}}$ is *time-independent*

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- **From Exponential to Ordered Exponential**
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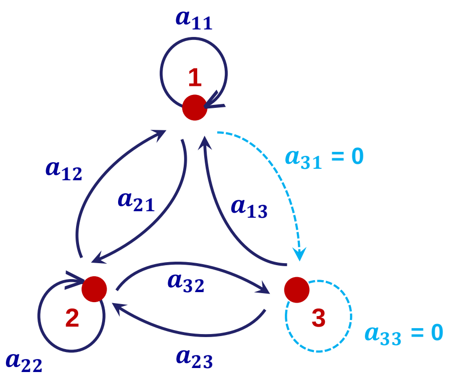
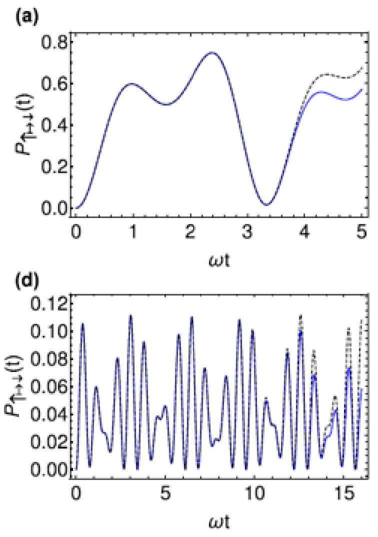




An intuitive interpretation of the Ordered Exponential (time depend. matrix)

- $\langle s_j | U(t) | s_i \rangle$ **corresponds to the sum of all walks $\mathcal{W}$ from $\mathcal{V}_i$ to $\mathcal{V}_j$ on $\mathcal{G}$ including all possible jumping times for each transition between vertices of $\mathcal{G}$**

ex.: consider the 3rd term of the Picard (Dyson) iteration:

→ $A(t_1)\, A(t_2)\, A(t_3)$

ex.: the {1,4} entry of the matrix reads:

→ $[A(t_1)\, A(t_2)\, A(t_3)]_{\{1,4\}} = \sum_{i,k} A(t_1)_{1,i}\, A(t_2)_{i,k}\, A(t_3)_{k,4}$

weight of 1 → i $\mathcal{E}$dge　　weight of i → k $\mathcal{E}$dge …

→ $\mathcal{W}$ from **1 to 4** of ***length* 3**

finally: time integration over t_1, t_2 and t_3: *all* $\mathcal{W}$, for *all* possible times, for *all* jumps between vertices

Ordered exponential

$$OE\left[A_{\mathcal{G}}\right](t',t) = \begin{pmatrix} \cdots \\ < s_j \left| OE[A_{\mathcal{G}}](t',t) \right| s_i > \\ \cdots \end{pmatrix}$$

Path-Sum

▶ resummation of all $\mathcal{W}$ involves a ***finite*** number of operations: ***sum*** *on* ***simple paths*** and ***continuous fraction*** *of* ***simple cycles*** with vertex removal

Σ **ALL *weighted* walks *j* ← *i* on A$_{\mathcal{G}}$**

but using $*$ –product

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

instead of ×

… and $[1_* - (* \;\; * \;\; * \cdots)]^{*-1} = \sum_{n\geq 0}(* \;\; * \;\; * \cdots)^{*n}$

Kernel, K

Neumann series (analytical)

Giscard, *J. Math. Phys.*, 2015

Time dependent 2 × 2 matrix

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

$$[1_* - (* \;\; * \;\; * \cdots)]^{*-1} = \sum_{n\geq 0} (* \;\; * \;\; * \cdots)^{*n}$$

Kernel, K

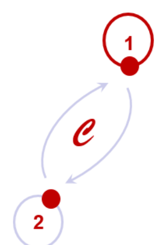
OE[A](t',t) = $\begin{pmatrix} \int_t^{t'} G_{K_2,11}(t',\tau)d\tau & OE_{12}(t',t) \\ OE_{21}(t',t) & \int_t^{t'} G_{K_2,22}(t',\tau)d\tau \end{pmatrix}$

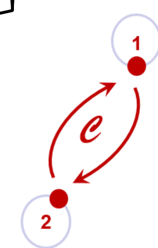
$a_{ij}(t)$

$$G_{K_2,11} = [1_* - a_{11} - a_{12} * G_{K_2\backslash\{1\},22} * a_{21}]^{*-1}$$

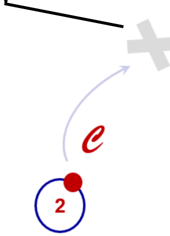
continuous fraction on *simple cycles*

$\mathcal{K}_2$



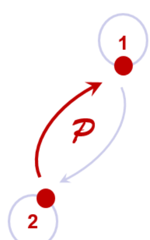


$$G_{K_2\backslash\{1\},22} = [1_* - a_{22}]^{*-1}$$



$$OE_{12}(t',t) = \int_t^{t'} G_{K_2\backslash\{2\},11} * a_{12} * G_{K_2,22}(t',\tau)d\tau$$

sum on *simple paths*



► **END !**

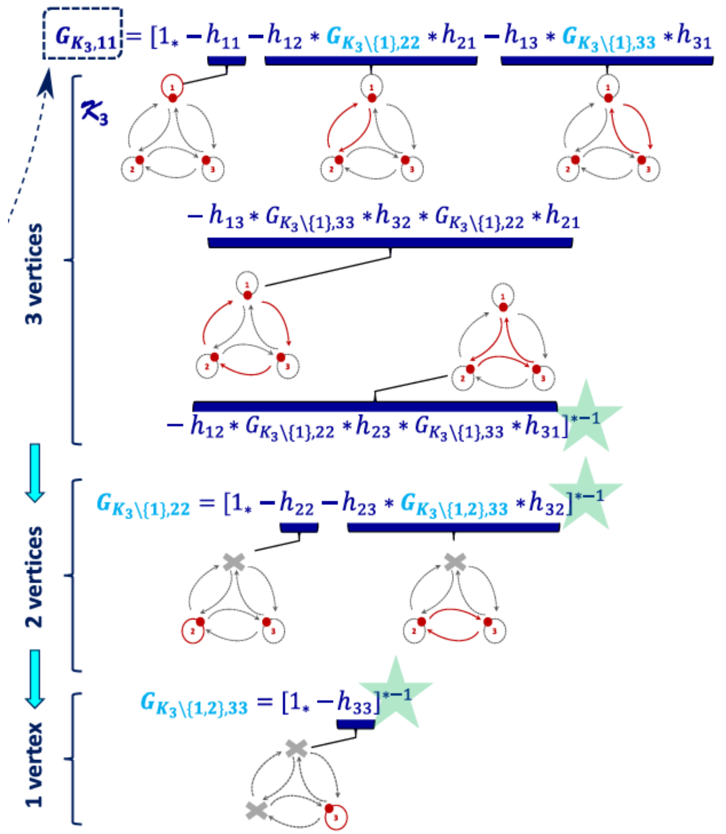
► ***finite*** sum on simple 𝒫

► **END** of the ***continued fraction !***

► ***finite*** sum on 𝒞

Summary (partial)

Path-Sum solution



► exact representation (transcendent, special functions…)

► non perturbative, super exponentially CV

► always closed form in

$$[1_* - (* \quad * \quad * \cdots)]^{*-1}$$

► Neumann series: analytic, closed form at fixed accuracy

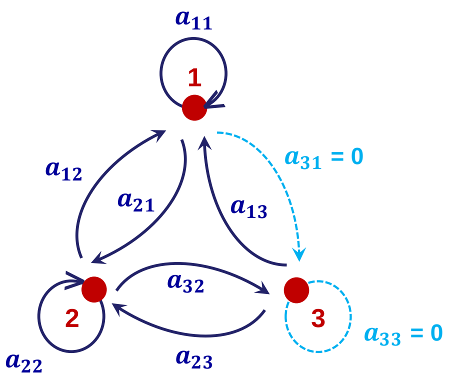
Outline

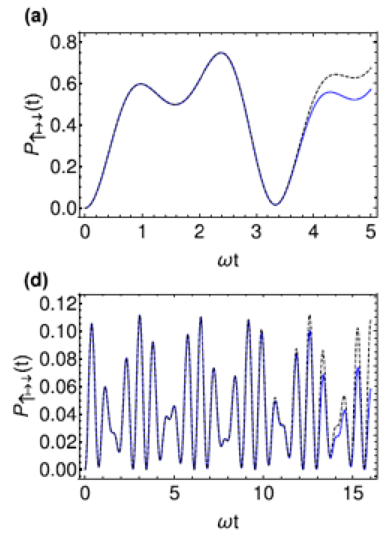
■ Introduction to Path-Sum

■ From Exponential to Ordered Exponential

■ **Analytical results**

■ Implementation in Mathematica





Linearly polarized excitation, Bloch-Siegert (BS) effect: analytical solution

Kernel K

entries of H(t)

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

$$K_\uparrow(t',t) = -ih_\uparrow(t') - \int_t^{t'}\int_{\tau_1}^{t'} h_{\uparrow\downarrow}(t')\big(\delta(\tau_2-\tau_1) - ih_\downarrow(\tau_2)\, e^{-i\int_{\tau_1}^{\tau_2} h_\downarrow(\tau_3)d\tau_3}\big) \times h_{\downarrow\uparrow}(\tau_1)d\tau_2 d\tau_1, \quad (6)$$

« shape » → Path-Sum

*–Resolvent

$$G_\uparrow := (1_* - K_\uparrow)^{*-1} = 1_* + \sum_{n>0} K_\uparrow^{*n}.$$

$$K_\uparrow^{*(n+1)} = \int_t^{t'} K_\uparrow^{*(n)}(t',\tau) K_\uparrow^{*}(\tau,t)\, d\tau$$

$$\mathsf{U}(t',t)_{\uparrow\uparrow} = \int_t^{t'} G_\uparrow(\tau,t)d\tau, \quad \mathsf{U}(t',t)_{\downarrow\downarrow} = \int_t^{t'} G_\downarrow(\tau,t)d\tau,$$

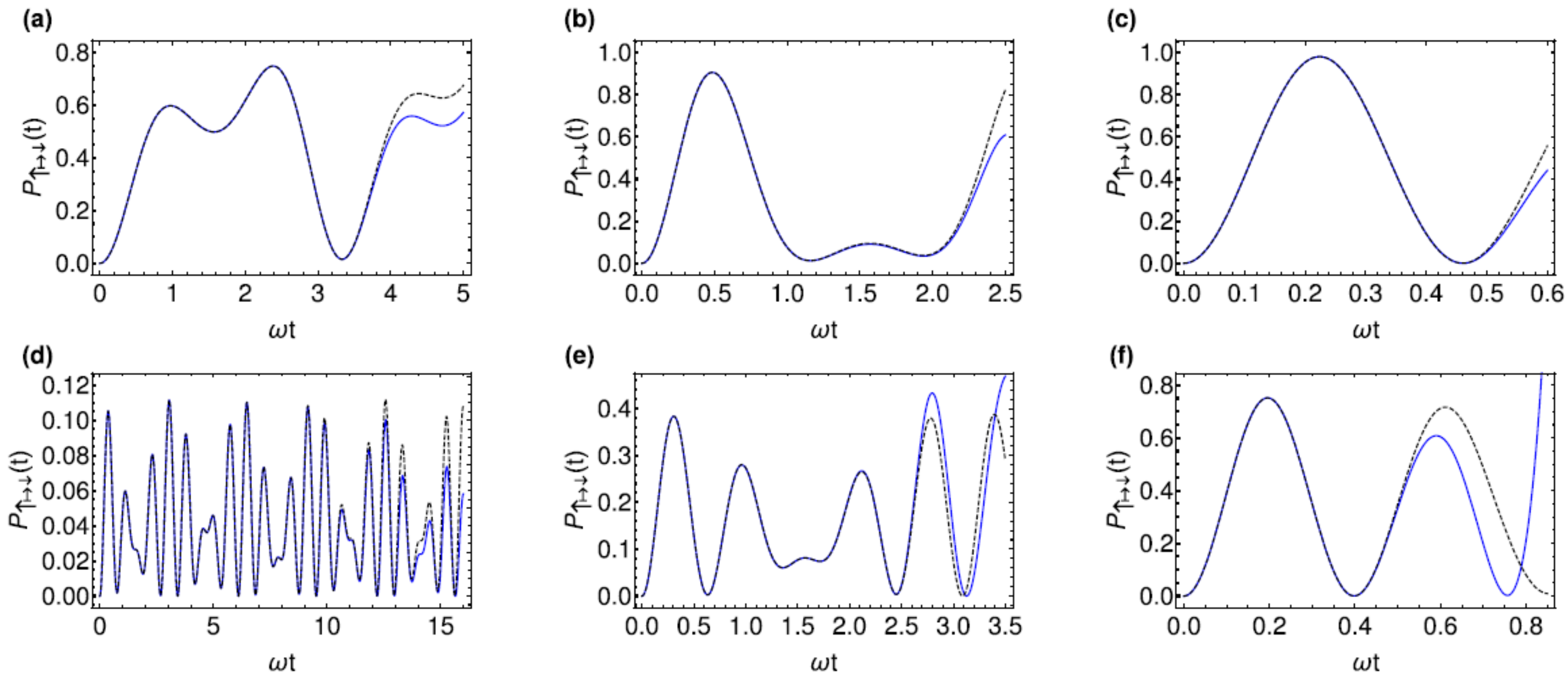
all individual entries of U(t) are now available

$\mathsf{U}(t',t)_{\downarrow\uparrow}$, $\mathsf{U}(t',t)_{\uparrow\downarrow}$ — above terms and simple paths

Linearly polarized excitation, Bloch-Siegert (BS) effect

► visualizing the solution at analytical / numerical level

P(t) transition probability



ON and OFF resonance

$\beta/\omega \ll 1$ *weak*

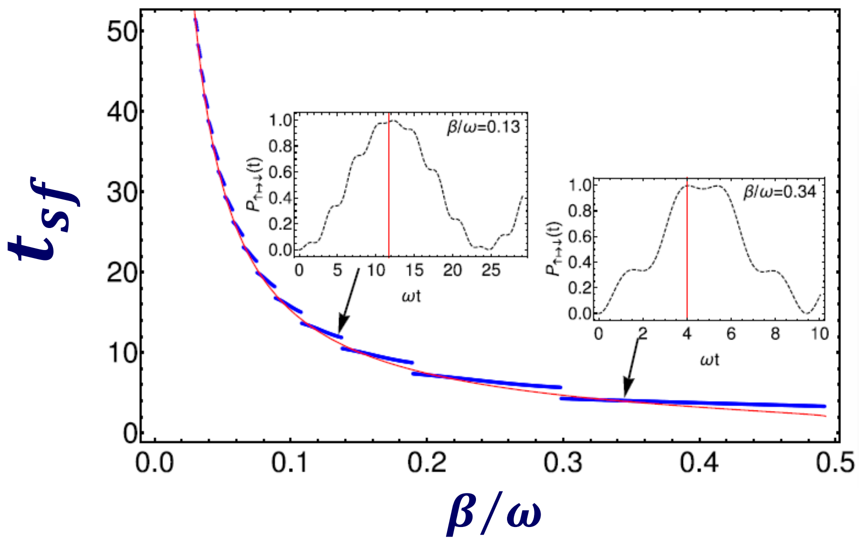
$\beta/\omega \gg 1$ *strong*

Giscard, Bonhomme, *Phys. Rev. Res.*, 2020

Linearly polarized excitation, Bloch-Siegert (BS) effect

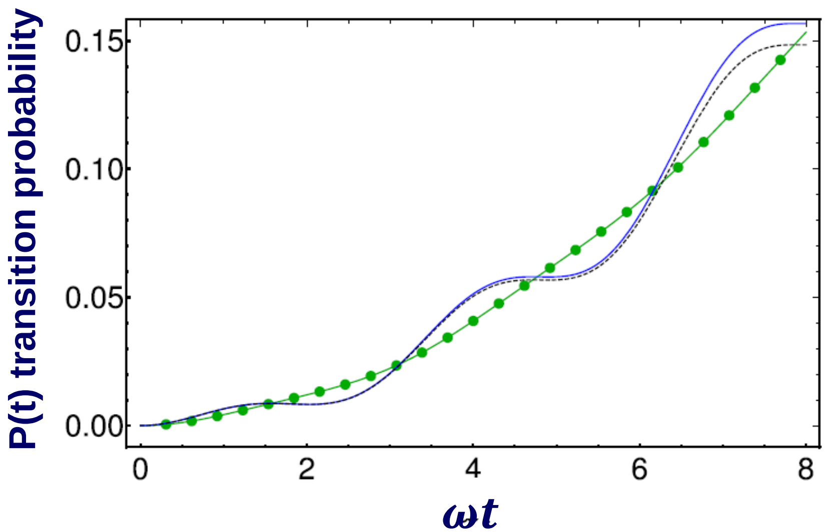
$$\mathbf{H}(t) = \begin{pmatrix} \frac{\omega_0}{2} & 2\beta\cos(\omega t) \\ 2\beta\cos(\omega t) & -\frac{\omega_0}{2} \end{pmatrix}$$

► analytical formula



spin flip duration, t_{sf}

$$t_{sf} = \frac{1}{2\sqrt{2}}\sqrt{\frac{12}{\beta^2} - \frac{15}{\omega^2} + \frac{\sqrt{3}}{\beta^4\omega^2}\sqrt{91\beta^8 - 88\beta^6\omega^2 + 16\beta^4\omega^4}}$$
$$= \frac{1}{\beta}\sqrt{\frac{1}{2}(3+\sqrt{3})} - \frac{\beta}{8\omega^2}\sqrt{\frac{1}{2}(129+67\sqrt{3})}$$
$$- \frac{\beta^3}{128\omega^4}\sqrt{\frac{1}{2}(16131+5545\sqrt{3})} + O(\beta^4). \qquad (11)$$



$\beta/\omega \ll 1$

order 0 of the Path-Sum solution

$$G_{\uparrow}^{(0)} = \delta(t', t)$$

$$P_{\uparrow\to\downarrow}^{(0)}(t) = \frac{\beta^2 t}{\omega}\sin(2\omega t) + \frac{\beta^2}{2\omega^2} + \beta^2 t^2 - \frac{\beta^2}{2\omega^2}\cos(2\omega t).$$

Separable (degenerate) kernel K

K (t', t)

$$G_{\alpha\alpha}(t',t) = [1_* - a_{\alpha\alpha} - a_{\alpha\omega} * [1_* - a_{\omega\omega}]^{*-1} * a_{\omega\alpha} - \cdots]^{*-1}$$

function of *one* time variable

separable

separable

$$K(t',t) := \sum_{i=1}^{d} K_i(t',t),$$

$$K_i(t',t) = a_i(t')b_i(t)$$

$$R_{K_i} := (1_* - K_i)^{*-1}$$

CLOSED–form

(Pleshchinski, Tagirov, J. Math. Sc., 1995)

► the solution of a linear Volterra equation of second kind with separable K is necessarily separable

conclusion: **K(t',t) is separable**

A fundamental consequence of separability: Accelarated Neumann Series

a series related to ORDINARY resolvents (here *u*, *v* are formal variables)

$$\frac{1}{1-u-v} = \frac{1}{1-u} \times \frac{1}{1-v} + \frac{uv}{(1-u)(1-v)} \times \frac{1}{1-u-v}$$

iteration…

formal series

$$\frac{1}{1-u-v} = \sum_{k=0}^{\infty} \frac{(uv)^k}{(1-u)^k(1-v)^k} \frac{1}{1-u} \frac{1}{1-v}$$

« accessible »

An interesting consequence of separability: Accelarated Neumann Series

a series related to ORDINARY resolvents (here *u*, *v* are formal variables)

$$\frac{1}{1-u-v} = \frac{1}{1-u} \times \frac{1}{1-v} + \frac{uv}{(1-u)(1-v)} \times \frac{1}{1-u-v}$$

iteration…

$$\frac{1}{1-u-v} = \sum_{k=0}^{\infty} \frac{(uv)^k}{(1-u)^k(1-v)^k} \frac{1}{1-u} \frac{1}{1-v}$$

« accessible »

$$R_K = \sum_{k=0}^{\infty} T^{*k} * \mathop{\Huge *}_{i=1}^{d} R_{K_i},$$

$$K(t',t) := \sum_{i=1}^{d} K_i(t',t),$$

$$K_i(t',t) = a_i(t')b_i(t)$$

$$R_{K_i} := \left(1_* - K_i\right)^{*-1}$$

CLOSED–form

- **extension to non–commutative *– product**
- **$R_K(t',t)$ in terms of $R_{K_i}(t',t)$ all accessible**
- **speed up of convergence if**

$$< T > = 0$$

Linearly polarized excitation, Bloch-Siegert (BS) effect

in the case of ultra-strong regime, *i.e.* $\beta/\omega_0 \gg 1$ and $< T > = 0$

$$K_1(t) = -2i\beta\begin{pmatrix} 0 & \cos(\omega t) \\ \cos(\omega t) & 0 \end{pmatrix}$$

$$K_2(t) = -i\omega_0\begin{pmatrix} 1/2 & 0 \\ 0 & -1/2 \end{pmatrix}.$$

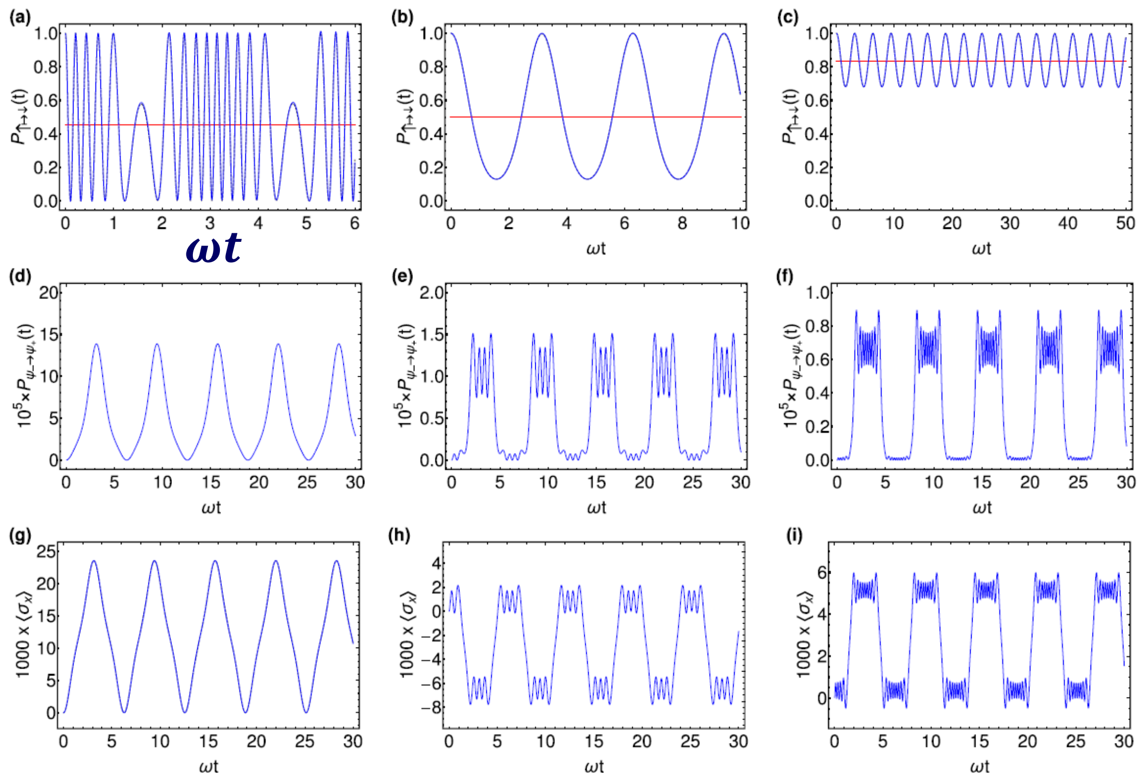
$$G^{(acc,0)}(t',t) = [U^{(acc,0)}(t',t)]'$$

$$= \int_t^{t'} \underbrace{G_1(t',\tau)G_2(\tau,t)d\tau}_{\text{related to individual } K_i}.$$

related to *individual* K_i

the first term of the Accelarated analytical Neumann Series is sufficient

ON and OFF resonance



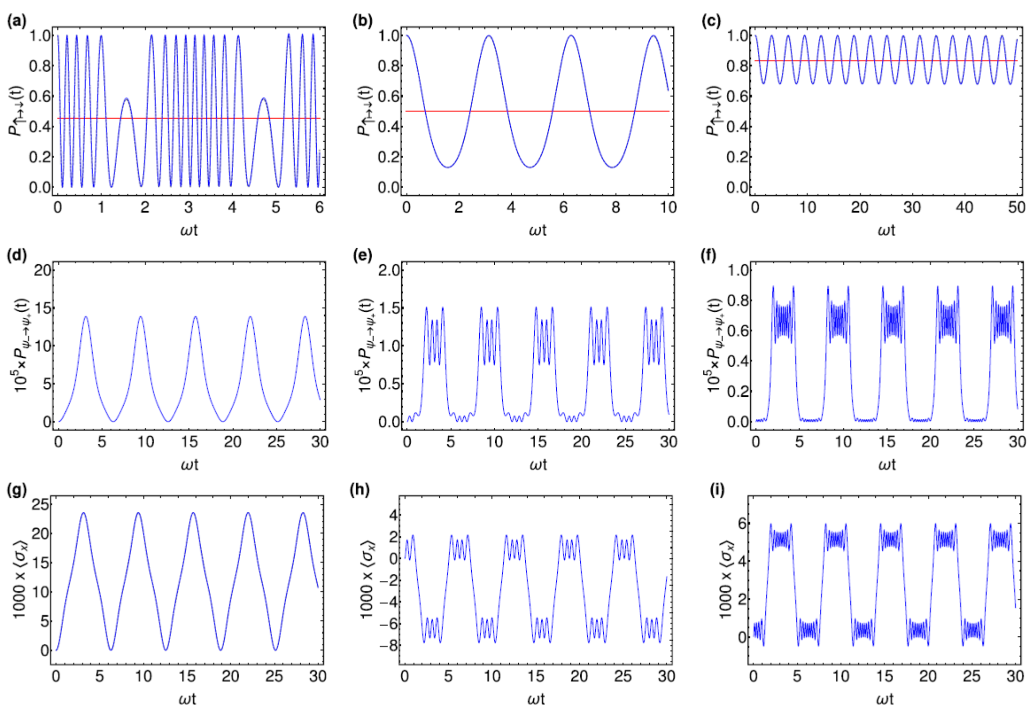
Giscard, *J. Integral Equations Appl*. 2020
Giscard, Bonhomme, *Phys. Rev. Res*. 2020

Linearly polarized excitation, Bloch-Siegert (BS) effect

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

Accelarated Neumann Series → **$\beta / \omega_0 >> 1$, $< T > = 0$**

$$\mathrm{U}^{(acc,0)}(t) = \begin{pmatrix} \cos\left(\frac{2\beta}{\omega}\sin(\omega t)\right) + e^{-\frac{1}{2}i\omega_0 t} - 1 & -i\sin\left(\frac{2\beta}{\omega}\sin(\omega t)\right) \\ -i\sin\left(\frac{2\beta}{\omega}\sin(\omega t)\right) & \cos\left(\frac{2\beta}{\omega}\sin(\omega t)\right) + e^{\frac{1}{2}i\omega_0 t} - 1 \end{pmatrix}$$
$$+ \int_0^t \begin{pmatrix} i\omega_0 e^{-\frac{1}{2}i\omega_0\tau}\sin^2\left(\frac{2\beta}{\omega}[\sin(\omega\tau) - \sin(\omega t)]\right) & -\frac{1}{2}\omega_0 e^{\frac{1}{2}i\omega_0\tau}\sin\left(\frac{4\beta}{\omega}[\sin(\omega\tau) - \sin(\omega t)]\right) \\ \frac{1}{2}\omega_0 e^{-\frac{1}{2}i\omega_0\tau}\sin\left(\frac{4\beta}{\omega}[\sin(\omega\tau) - \sin(\omega t)]\right) & -i\omega_0 e^{\frac{1}{2}i\omega_0\tau}\sin^2\left(\frac{2\beta}{\omega}[\sin(\omega\tau) - \sin(\omega t)]\right) \end{pmatrix} d\tau.$$

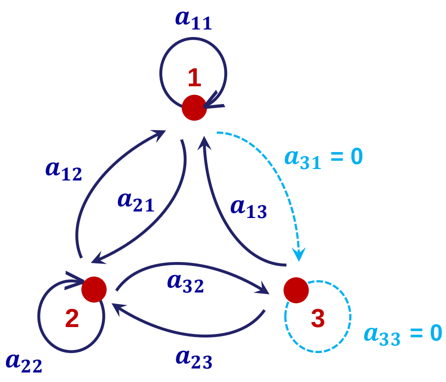


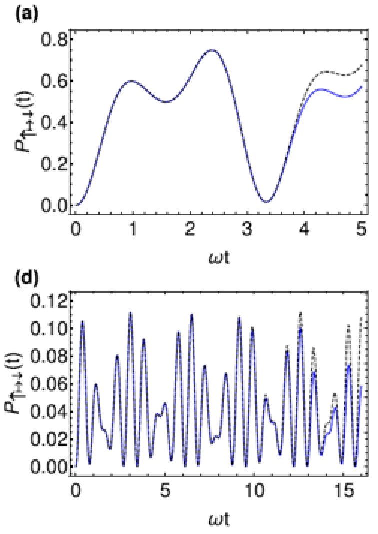
$< T > = 0$

▶ **predictions**

Outline

- Introduction to Path-Sum
- From Exponential to Ordered Exponential
- Analytical results
- **Implementation in Mathematica**





Implementation in Mathematica

$$\hat{\hat{L}}_{\mathrm{B}}(t) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ s^{\mathrm{eq}}_{\mathrm{a},z}(t)/T_1^{\mathrm{e}} & -1/T_1^{\mathrm{e}} & \omega_1 & 0 & 0 & 0 & 0 & DJ_{\mathrm{ab}}(t) & 0 & 0 \\ 0 & -\omega_1 & -1/T_2^{\mathrm{e}} & -\Delta\omega_{\mathrm{a}}(t) & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -\Delta\omega_{\mathrm{a}}(t) & -1/T_2^{\mathrm{e}} & 0 & 0 & 0 & 0 & 0 & 0 \\ s^{\mathrm{eq}}_{\mathrm{b},z}(t)/T_1^{\mathrm{e}} & 0 & 0 & 0 & -1/T_1^{\mathrm{e}} & \omega_1 & 0 & -DJ_{\mathrm{ab}}(t) & 0 & 0 \\ 0 & 0 & 0 & 0 & -\omega_1 & -1/T_2^{\mathrm{e}} & -\Delta\omega_{\mathrm{b}}(t) & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -\Delta\omega_{\mathrm{b}}(t) & -1/T_2^{\mathrm{e}} & 0 & 0 & 0 \\ 0 & -DJ_{\mathrm{ab}}(t)/2 & 0 & 0 & DJ_{\mathrm{ab}}(t)/2 & 0 & 0 & -1/T^{\mathrm{e}}_{2,\mathrm{ZQ}} & -\Delta\omega_{\mathrm{D}}(t) & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \Delta\omega_{\mathrm{D}}(t) & 0 & 0 \\ s^{\mathrm{eq}}_{\mathrm{n},z}/T_1^{\mathrm{n}} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1/T_1^{\mathrm{n}} \end{bmatrix}$$

```
In[•]:= A = {
0 0 0 0 0 0 0 0 0 0
1 1 1 0 0 0 0 1 0 0
0 1 1 1 0 0 0 0 0 0
0 0 1 1 0 0 0 0 0 0
1 0 0 0 1 1 0 1 0 0
0 0 0 0 1 1 1 0 0 0
0 0 0 0 0 1 1 0 0 0
0 1 0 0 1 0 0 1 1 0
0 0 0 0 0 0 0 1 0 0
1 0 0 0 0 0 0 0 0 1 };
```

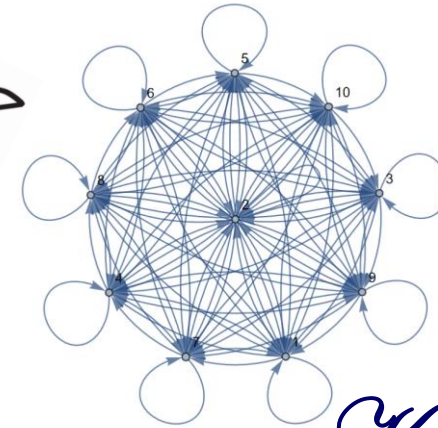
t dependent matrix (*sparse*)

μw, D–J events, relaxation times…

in: DNP simulations

see: F. Mentink-Vigier *et al., PCCP*, 2017

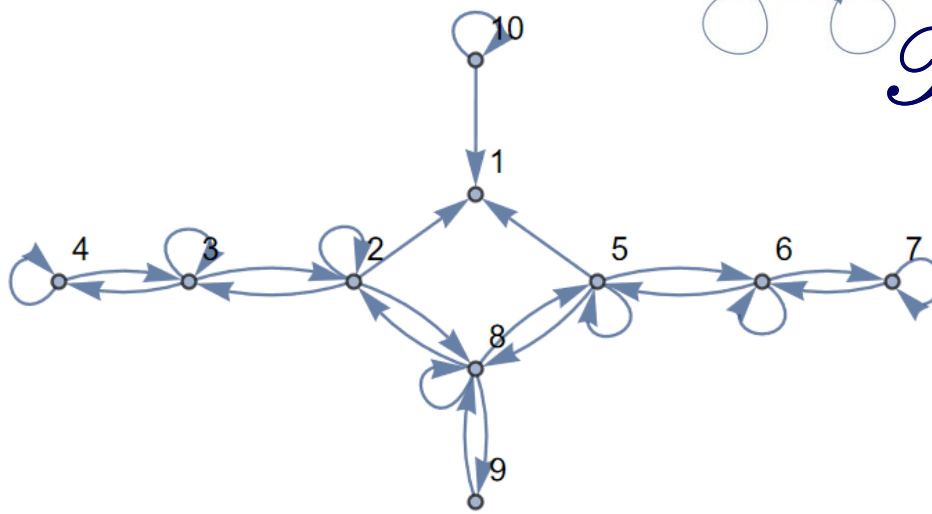
Implementation in Mathematica



$\mathcal{K}_{10}$

entries: 1 × 1 matrices

```
In[•]:= A = 
0 0 0 0 0 0 0 0 0 0
1 1 1 0 0 0 0 1 0 0
0 1 1 1 0 0 0 0 0 0
0 0 1 1 0 0 0 0 0 0
1 0 0 0 1 1 0 1 0 0
0 0 0 0 1 1 1 0 0 0 ;
0 0 0 0 0 1 1 0 0 0
0 1 0 0 1 0 0 1 1 0
0 0 0 0 0 0 0 1 0 0
1 0 0 0 0 0 0 0 0 1
```




```
In[•]:= (*PATH SUM MODULES;
     PrimeSet : returns the prime set of a walk;
     PathsGen : gives all the primes of a prime set that are from vertex i to vertex j;
     Cycle : gives all the prime cycles off a given vertex,
     that are given in a given prime set and do not cross a specified set of vertices;
     WDVertex: gives weighted dressed vertices;
     WPathSum: gives weighted prime paths;
     RandomPrimeList: generates a list of simple cycles and simple paths by factoring random walks.
```

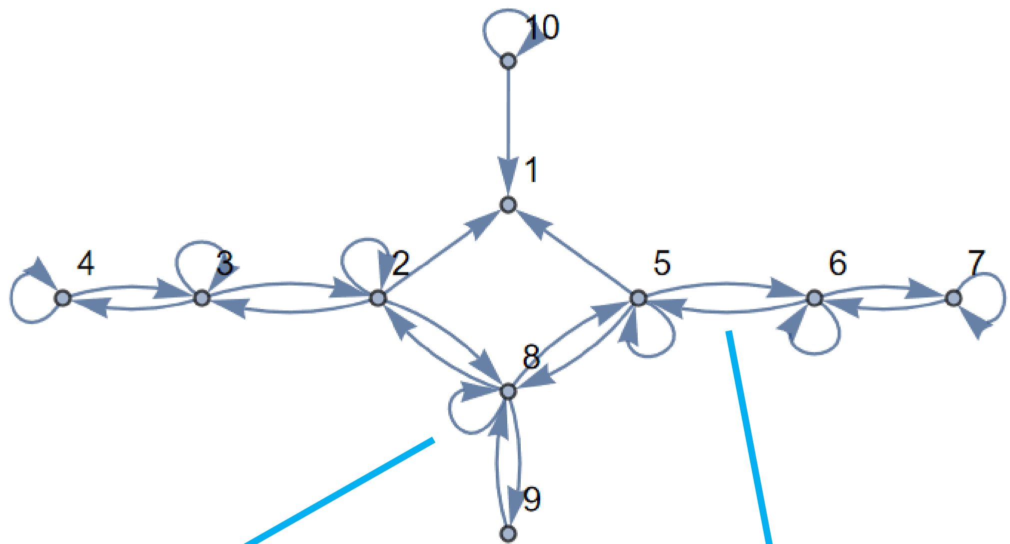
→ factors random walks, gives simple cycles and paths, constructs the Path-Sum for all entries of a *given* partition

Implementation in Mathematica

In[•]:= A =

0	0	0	0	0	0	0	0	0	0
1	1	1	0	0	0	0	1	0	0
0	1	1	1	0	0	0	0	0	0
0	0	1	1	0	0	0	0	0	0
1	0	0	0	1	1	0	1	0	0
0	0	0	0	1	1	1	0	0	0
0	0	0	0	0	1	1	0	0	0
0	1	0	0	1	0	0	1	1	0
0	0	0	0	0	0	0	1	0	0
1	0	0	0	0	0	0	0	0	1

;



OE[A(t',t)] (*– products):

entry {8,8}

$$\frac{1}{1 - z - z^2 - \frac{2 z^2}{1-z-\frac{z^2}{1-z-\frac{z^2}{1-z}}}}$$

entry {5,6}

$$\frac{z}{\left(1 - z - \frac{z^2}{1-z}\right) \times \left(1 - z - \frac{z^2}{1-z-\frac{z^2}{1-z}} - \frac{z^2}{1-z-z^2-\frac{z^2}{1-z-\frac{z^2}{1-z-\frac{z^2}{1-z}}}}\right)}$$

Path-Sum

- ► a new approach
- ► analytical expression for U(t)
- ► convergence
- ► non perturbative formulation
- ► partitions and scalability
- ► other theory/applications to come…

P.-L. Giscard

S. Pozza

anr agence nationale de la recherche

Proposition 3.1. *Let $I \subset \mathbb{R}$ and let $(t', t) \in I^2$ be two variables and let $g(t', t)$ be a generalized function of t', t. Let $f(t', t) = \tilde{f}(t', t)\Theta(t' - t)$ be a function of t', t over I^2 and $K(t', t) := \tilde{a}(t')\tilde{b}(t)\Theta(t' - t)$. Let $\tilde{\alpha} := \int \tilde{K}(\tau, \tau)d\tau = \int \tilde{a}(\tau)\tilde{b}(\tau)d\tau$. Then the solution f of the linear*

Volterra equation of the second kind $f = g + K * f$ with kernel K is

$$f(t', t) = g(t', t) +$$

$$\tilde{a}(t') \int_{-\infty}^{\infty} \tilde{b}(\tau) \exp\left(\int_{\tau}^{t'} \tilde{a}(\tau')\tilde{b}(\tau')d\tau' \right) \Theta(t' - \tau) g(\tau, t)\, d\tau. \tag{10}$$

***Remark* 3.1.** *In the (typical) case where g itself takes on the form $g(t', t) = \tilde{g}(t', t)\Theta(t' - t)$, in the expression of Eq. (10), $g(\tau, t)$ can be replaced with $\tilde{g}(\tau, t)$ with the outer integral running from t to t'. If instead one chooses $g(t', t) = \delta(t' - t)$, then the Volterra equation satisfied by f reads $f = 1_* + K * f$, that is f is the $*$-resolvent of K, $f = R_K$ and Eq. (10) simplifies to*

$$\begin{aligned} R_K(t', t) &= \delta(t' - t) + \tilde{a}(t')\tilde{b}(t)e^{\tilde{\alpha}(t') - \tilde{\alpha}(t)}\Theta(t' - t) \\ &= \delta(t' - t) + \tilde{K}(t', t)e^{\tilde{\alpha}(t') - \tilde{\alpha}(t)}\Theta(t' - t). \end{aligned}$$

In other terms, the $*$-resolvent of a kernel of the form $K(t', t) = \tilde{a}(t')\tilde{b}(t)\Theta(t' - t)$ is exactly available in closed form.

Proof. We proceed by induction on the Neumann series $f = \left(\sum_n K^{*n}\right) * g$. Convergence of this series is guaranteed whenever $\tilde{a}$ and $\tilde{b}$ are bounded over all compact subintervals of I, however existence of the final form for f is clearly independent from this assumption. In this situation this form can be understood as the analytic continuation of the original Neumann series.

Other applications in NMR

Exact solutions for the time-evolution of quantum spin systems under arbitrary waveforms using algebraic graph theory

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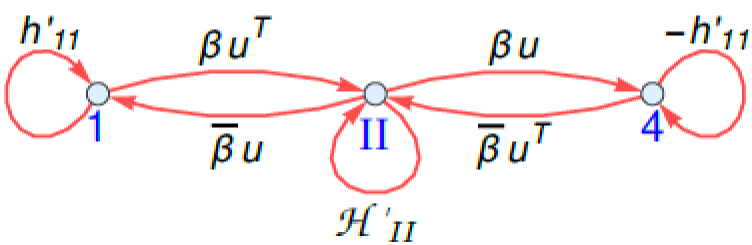
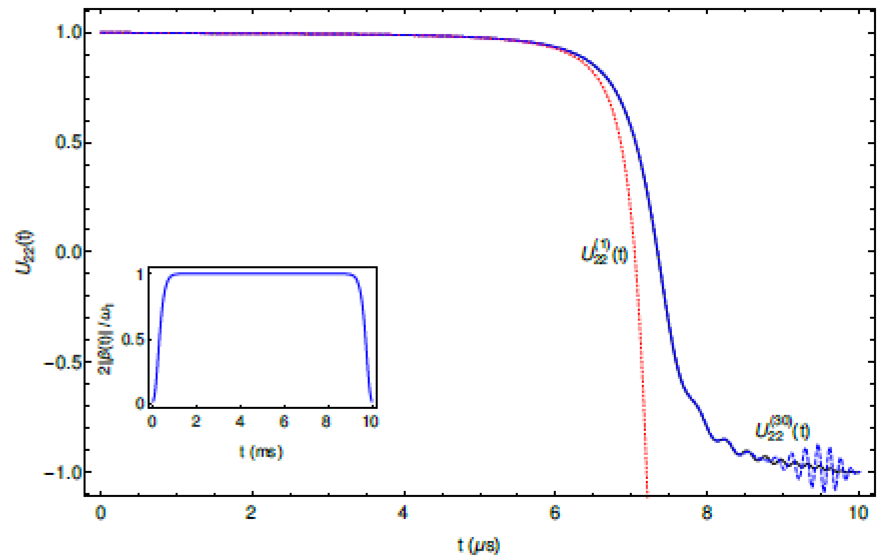


Figure 2: Graph $G_{\mathscr{H}'}$ showing the structure of the quantum state space as imposed by the bipartite Hamiltonian $\mathscr{H}'$ when partitioned as per eq. (24). Because the structure of $G_{\mathscr{H}'}$ and of the monopartite Hamiltonian graph $G_{\mathscr{H}}$ of Figure 1 differ only in the presence of a central loop on vertex 2, the path-sum formulation of the corresponding evolution operators will differ only in a single term representing this loop.



Cite as: arXiv:2205.05195 **[quant-ph]**

(or arXiv:2205.05195v1 **[quant-ph]** for this version)

https://doi.org/10.48550/arXiv.2205.05195

Numerical implementation for small matrices

- The Volterra composition *

$$(f * g)(t', t) = \Theta(t' - t) \int_t^{t'} \tilde{f}(t', \tau)\tilde{g}(\tau, t) d\tau$$

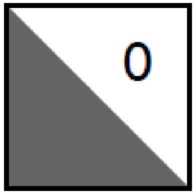
discretize t

$$(f * g)(t', t) \simeq \sum_{i \geq j \geq k} \underbrace{f(t_i, t_j) g(t_j, t_k) \Delta t}_{F_{ij}.G_{jk}\,\Delta t}$$

the key point

Matrix product !

Triangular matrices



- *-inverses : ordinary inverses of triangular matrices

well-conditioned (always)

Heun functions (Giscard *et al*., , *IEEE*, 2021)

- **newly implemented in**

- version 12)

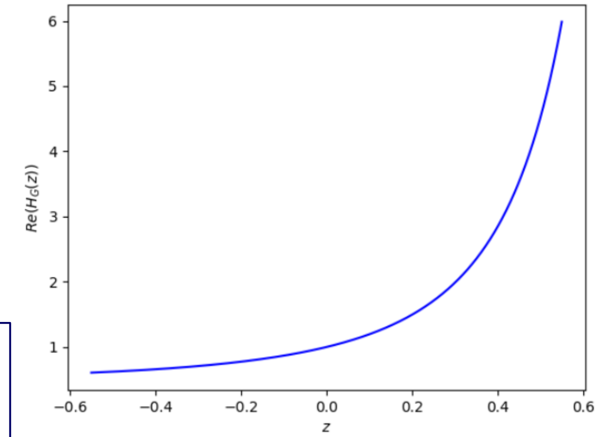
$$\frac{d^2H_G(z)}{dz^2}+\left[\frac{\gamma}{z}+\frac{\delta}{z-1}+\frac{\epsilon}{z-t}\right]\frac{dH_G(z)}{dz}+\frac{\alpha\beta z-q}{z(z-1)(z-t)}H_G(z)=0$$

$-B_1(z)$ $\qquad -B_2(z)$

Algebra

$$\mathsf{M}(z)=\begin{pmatrix} \frac{1}{B_1(z)+B_2(z)-1} & \frac{1}{B_1(z)-1} \end{pmatrix}$$

$$\frac{d}{dz}\mathsf{U}(z)=\mathsf{M}(z)\mathsf{U}(z)$$



Code	N	Time (sec.)
HeunG	1000	2.22
Python	1000	0.0096
HeunG	10000	22.4
Python	10000	0.090
HeunG	50000	110.8
Python	50000	0.43
HeunG	100000	231
Python	100000	0.90
HeunG	200000	464
Python	200000	1.87

- **accuracy ~ 10^{-6} (…towards Gauss quadrature ~ 10^{-16})**
- **… beats standard ODE solver with same number of points**
- **>> Zassenhaus (even for small matrices…)**

Path-Sum *vs* other methods

▶ main goal → get an ***exact*** form for ***U(t)***

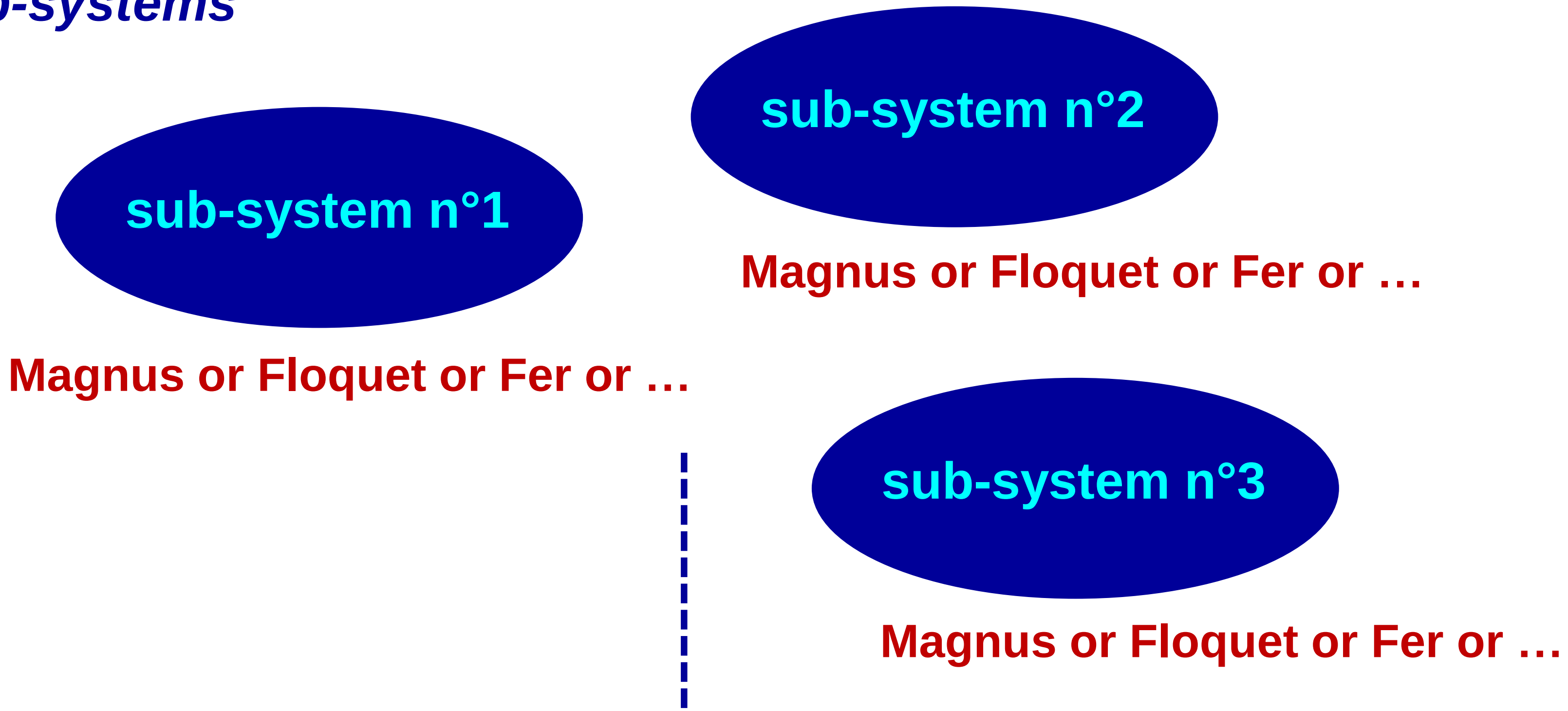
▶ **FLOQUET** | **ZASSENHAUS** **FER/TROTTER-SUZUKI** | **MAGNUS** | **PATH-SUM**

▶ usually:  on ***H(t)*** → choice in **FLOQUET** | **ZASSENHAUS** **FER/TROTTER-SUZUKI** | **MAGNUS**

▶ **PATH-SUM** is ***exact*** and **PARTITIONS** allow to ***choose the dimension*** of the working space from ***H(t)*** to ***U(t)***

Scale invariance

Take a **partition** of a spin system in a set of (***smaller***, ***independent***) ***sub-systems***



the ***exact*** evolution of the ***entire*** spin system as functions of the evolutions of the ***isolated sub-systems*** is given by **Path-Sum**

(though **non contiguous blocks** in H(t) matrix!)

WHY does Path-Sum work?

► the ***EXACT*** result is given by a ***FINITE*** number of terms

► the ***matrix*** nature of the problem is ***fully replaced*** when working on ***entries***

► or, one can keep it partially… → **PARTITIONS**

► ***hard*** work → $[\mathbf{1}_* - (* \;\; * \;\; * \cdots)]^{*-1}$

► hopefully: the ***Neumann series*** give the analytical solution at any order with unconditional convergence (not to be “found” … just apply a "recipe")

► the ***convergence*** of the Neumann series is ***superexponential***

► a ***convenient*** numerical approach: linear ***Volterra*** equations (***2^{nd} kind***)

$$D_x^2\, u + \left[\frac{\gamma}{x} + \frac{\delta}{x-1} + \frac{\epsilon}{x-a}\right] D_x u + \left[\frac{\alpha\beta\, x - q}{x(x-1)(x-a)}\right] u = 0$$

ex.: the best obtainable solution for the ***general 2 × 2 matrix*** (closed form for the ***confluent Heun’s special functions***) (see Q. Xie, 2018)

Exponential explosions

► **1st** explosion: related to the ***size of H(t)*** with ***many-body*** systems (Q nature)

► **2nd** explosion: related to the ***time*** needed to isolate the ***primes*** ($\mathcal{G}$ nature)

Lanczos–Path-Sum (numerical) ***fixes*** the **2nd** explosion:

Idea behind: initial H(t) → time dependent ***tridiagonal matrix***

expectations: to reach ***excellent convergence*** with the breadth of the continued fraction and why not ?... "Circumvent" the **1st** explosion

► for ***finite*** $\mathcal{G}$ **:** the decomposition of $\mathcal{W}$ in ***primes*** (e.g. ***simple paths*** & ***cycles***) for the ◘ (***nested***) operation ***exists and is unique***

► to determine the existence of a prime of ***length L*** is ***NP-complete*** (***no*****(?)** algorithm with polynomial complexity)

► to ***count*** them is ***#P-complete*** (the same but for counting problems)

► to count them for a fixed ***length L*** is ***#W[1]-complete*** (same as *#P-complete* but with parameters, such as *L*, taken into account)

► **BUT**: for ***sparse*** $\mathcal{G}$: counting becomes ***polynomial*** in the max degree of $\mathcal{G}$ **!**

see: **P. L. Giscard *et al., Algorithmica*, 2019**

Mathematical conditions on A(t) for Path-Sum to be valid -1

► fundamentally: $\mathcal{R}_{esolvent}[\mathbf{A(t)}]_{\ast\ \mathbf{product}} = \frac{\mathbf{d}}{\mathbf{dt}}\mathbf{OE}[\mathbf{A}(\mathbf{t})] \rightarrow$ **Path-Sum**

► each ***entry*** of A(t) must be ***bounded*** on [0,t], a ***bounded*** interval of time

► if the entries are ***not bounded***, Path-Sum still work … but perhaps the Neumann series will ***not converge***

► ***continuity*** is ***not*** necessary

► ***if continuity***: Volterra equations are much ***easier*** to handle

► A(t) can be Hermitian ***or not***, periodic ***or not …*** and entries can be: matrices, quaternions, octonions, division rings…

Mathematical conditions on A(t) for Path-Sum to be valid -2

► ***finite*** A(t): ***sufficient*** condition for ***finite breadth*** of the continued fraction

► ***NOT*** a ***necessary*** condition: ex. a ***finite*** number of ***simples cycles*** in an ***infinite*** matrix

► in some cases, Path-Sum can still be applied on ***infinite matrices***: ***strong symmetry***, e.g. invariance by translation (soluble ***non-linear*** Volterra equations)

In other words:

■ ***infinity*** of cycles … but ***self-similar*** like in a ***fractal***

■ the corresponding continued fraction is of ***finite breadth***

► take one entry: $\mathrm{f(t) = OE[A(t)]_{ij}}$

► ***Taylor*** series: expansion in t^n *i.e.* $f(t) = \sum_{n=0}^{\infty} \frac{f^{(n)}(0)}{n!} t^n$

ex.: $\frac{1}{1-t} = \sum_{n=0}^{\infty} t^n = 1 + t + t^2 + \cdots + t^n + \cdots$ with **r = 1** (***radius of CV***)

► ***Neumann*** series: uses the $*$ −**product**, i.e. $f(t) = \sum_{n=0}^{\infty} f^{*n}$

each order contains functions represented by intinite Taylor series

r = ∞ **(!)** with ***uniform*** & ***superexponential*** CV

N spins starting with a pure state

► starting with a ***pure state*** with ***1*** up-spin (total: **N**, ***any geometry***)

Path-sum contains all ***N-order correlations***

→ **if** $\boldsymbol{\omega_{rot} = 0}$

all terms of the Neumann series are ***explicitly*** known

→ **if** $\boldsymbol{\omega_{rot} \neq 0}$

still ***analytical*** up to the CV of the series to the solution

► starting with a ***pure state*** with ***4 or 5*** up-spin is still tractable

(*i.e.* no exponential explosion)

Pure state *vs* partial polarization

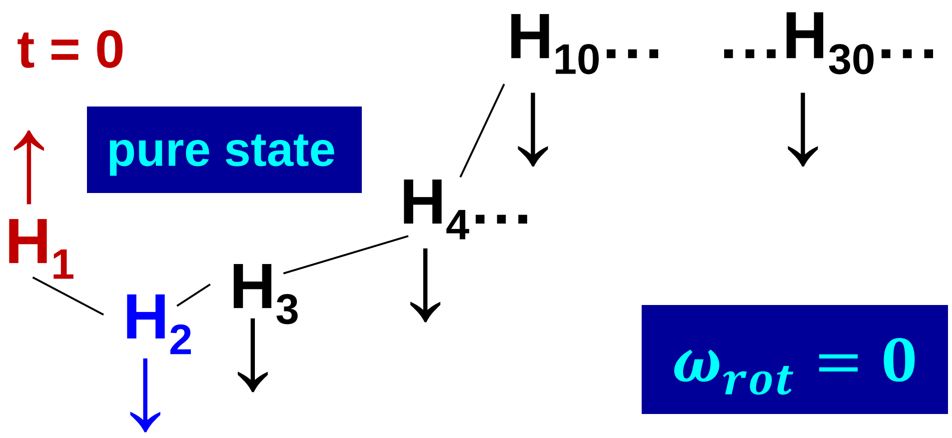
► **Pure state**: if ***k* up-spins** over N and ***k* << *N*** → space of states dim. ≈ $\boldsymbol{N^k}$ (suppression of the exponential explosion)

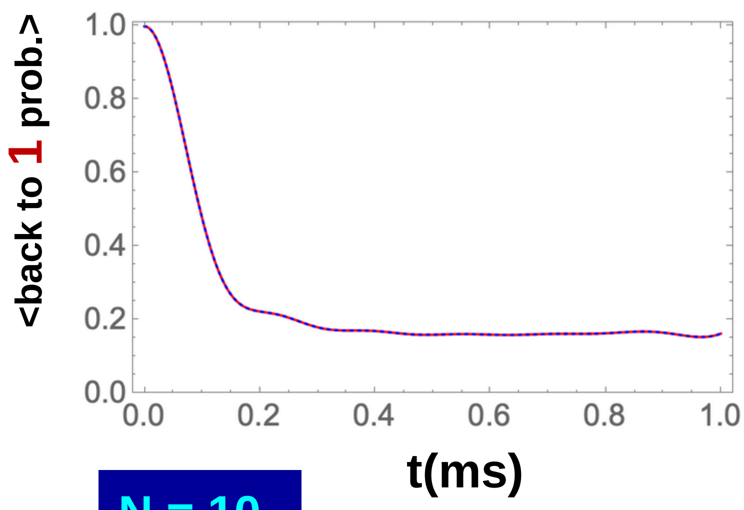
► **Partial polarization**: a ***cut-off*** is needed → if $\left|\frac{int_{i,j}}{intV} \le \frac{1}{cut\!-\!off}\right|$ then $int_{i,j}$= 0

cut-off **:** « high » for ***chains*** but decreases for more ***« dense »*** spin systems

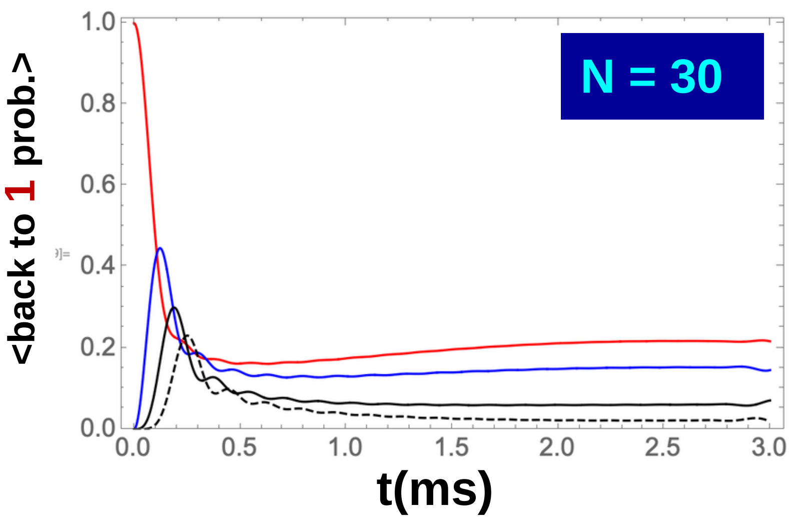
next target: to extend **Path-Sum** to **mixed states** *via* a **decomposition on pure states**

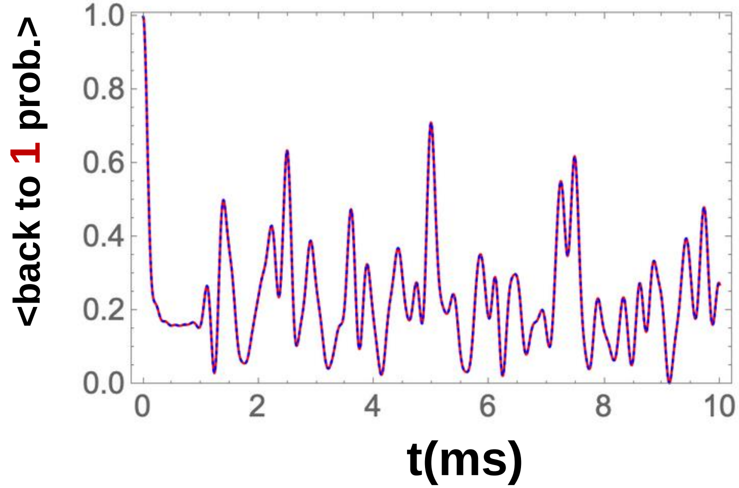
N spin chains and H_D





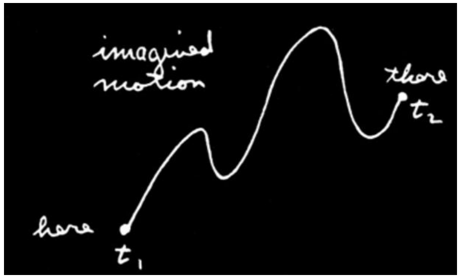
N = 10





P.-L. Giscard, C. Bonhomme, ArXiv 2019

Feynman paths and diagrams



*« With application to quantum mechanics, path integrals suffer most grievously from a serious defect. They do not permit a discussion of spin operators or other such operators in a simple and lucid way » (**R.P. Feynman**)*

► Path-sum can be used starting from the ***Lagrangian*** with ***action*** as ***weight*** on a given $\mathcal{W}$

► Path-sum can be used starting from the ***Hamiltonian*** with ***energy*** as ***weight*** on a given $\mathcal{W}$

► ***Feynman diagrams***: $\mathcal{W}$ of $\mathcal{G}$ in the state space (but ***continuous***)

► Path-sum performs a formal **re-summation** of an infinite number of $\mathcal{W}$, *i.e.* Feynman diagrams !

Numerical implementation for larger matrices

Lanczos algorithm → classical tridiagonalization

$*$– Lanczos Path-Sum algorithm

Pozza, Giscard
2020- 2022

full

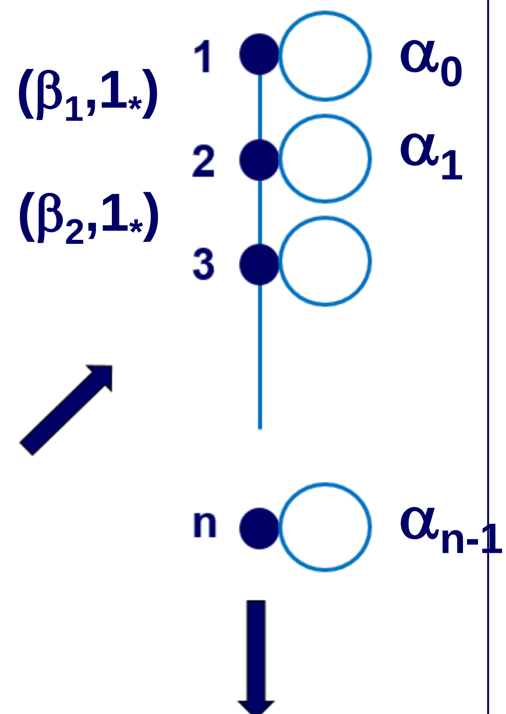
$$A(t') = \begin{pmatrix} a(t') & b(t') & \dots \\ c(t') & \dots & \dots \\ \dots & \dots & \dots \end{pmatrix} \quad N \times N$$

$*$– Lanczos

tridiagonal

$$T_n(t') = \begin{pmatrix} \alpha_0(t') & 1_* & & \\ \beta_1(t') & \alpha_1(t') & \ddots & \\ & \ddots & \ddots & 1_* \\ & & \beta_{n-1}(t') & \alpha_{n-1}(t') \end{pmatrix}$$

n << N



a very simple continued fraction to handle !

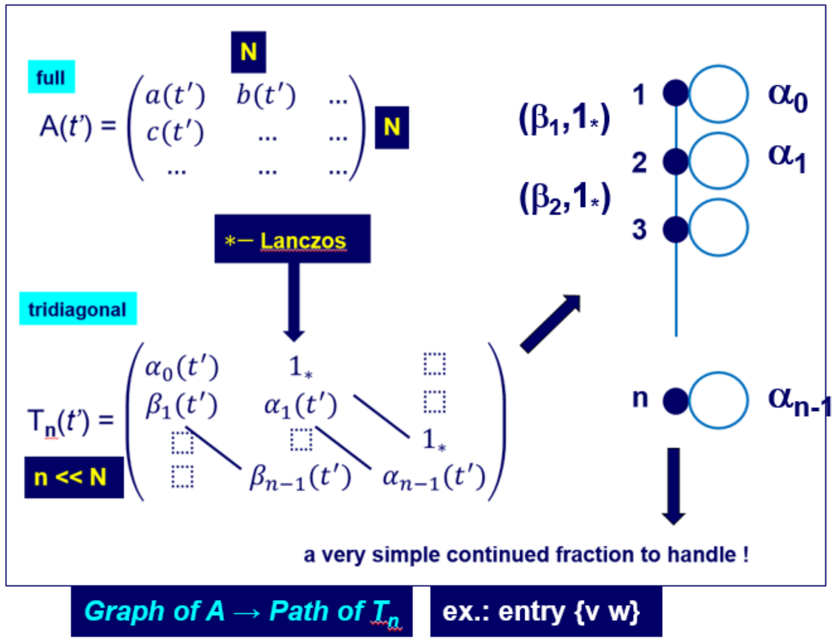
Graph of A → Path of T_n

ex.: entry {v w}

Numerical implementation for larger matrices

Matching Moment Property

$$w^H (\mathsf{A}^{*j})\, v = e_1^H (\mathsf{T}_n^{*j})\, e_1, \quad for \quad j = 0, \ldots, 2n-1$$



approximation of individual entry

$$w^H \mathsf{U}(t',t)\, v \approx e_1^H \mathsf{U}_n(t',t)\, e_1 = \Theta(t'-t) \int_t^{t'} \mathsf{R}_*(\mathsf{T}_n)_{1,1}(\tau,t)\, \mathrm{d}\tau;$$

$$\mathsf{R}_*(\mathsf{T}_n)_{1,1}(t',t) = \left(1_* - \alpha_0 - \left(1_* - \alpha_1 - (1_* - \ldots)^{*-1} * \beta_2\right)^{*-1} * \beta_1\right)^{*-1},$$