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Dynamics of NV centres interacting with background spins

ICQ seminar talk

Outline

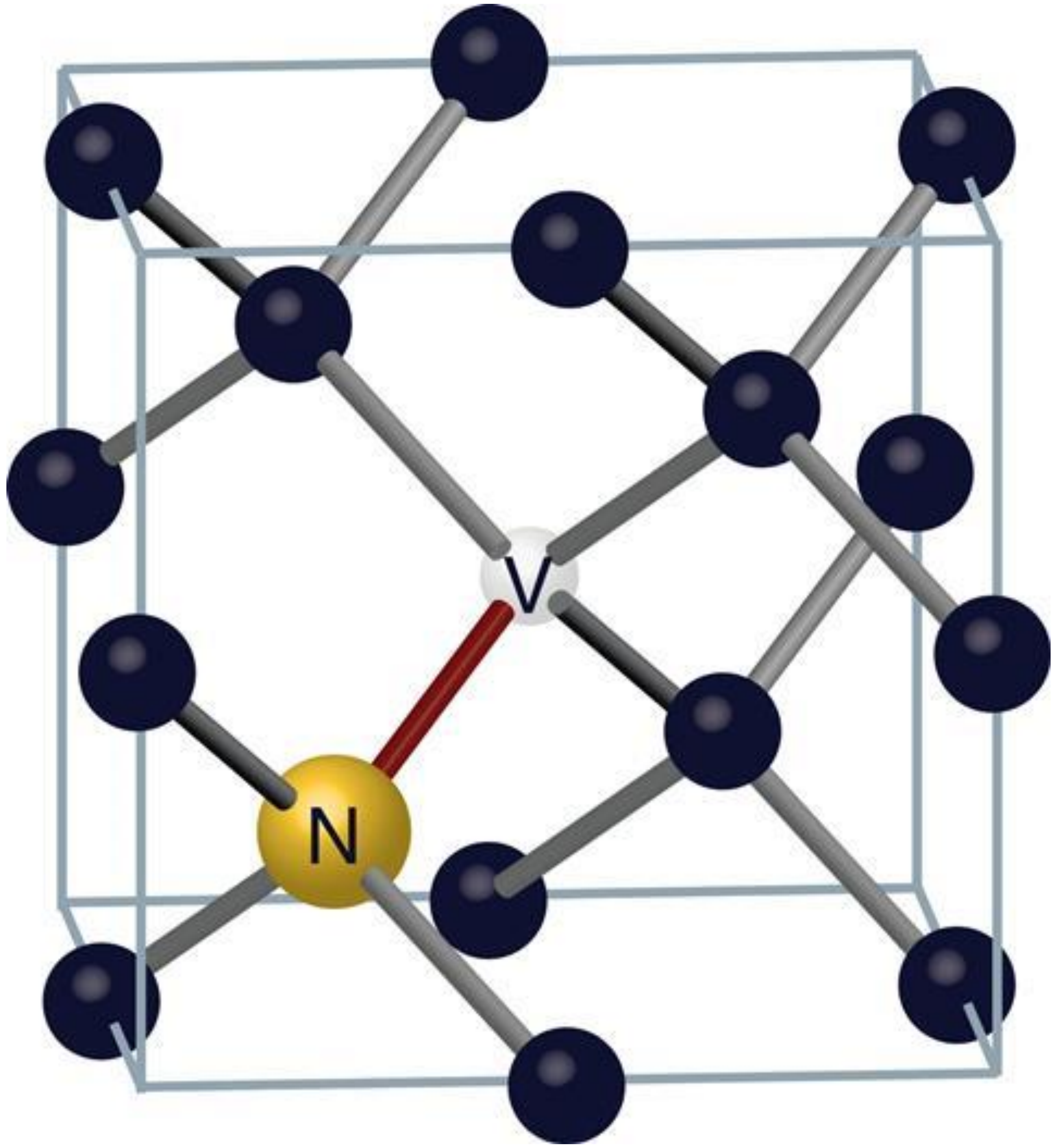
I. The Nitrogen Vacancy & motivation

II. The model

III. Summary

IV. Outlook & next steps

The NV center & motivation



- longest coherence time at room temperature[1]

$(2{,}43 \pm 0{,}06)$ ms

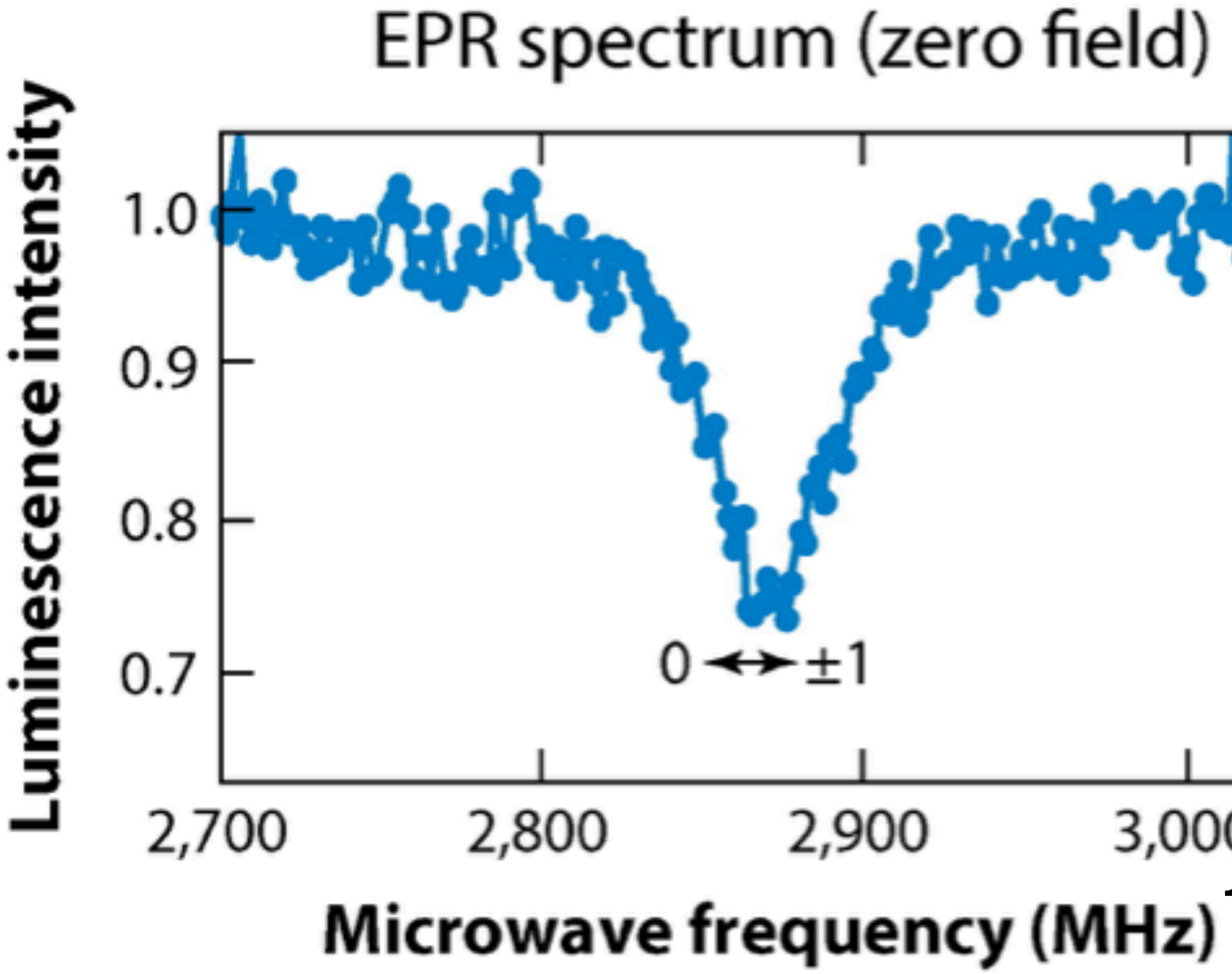
→ single photon source

→ potential for quantum information

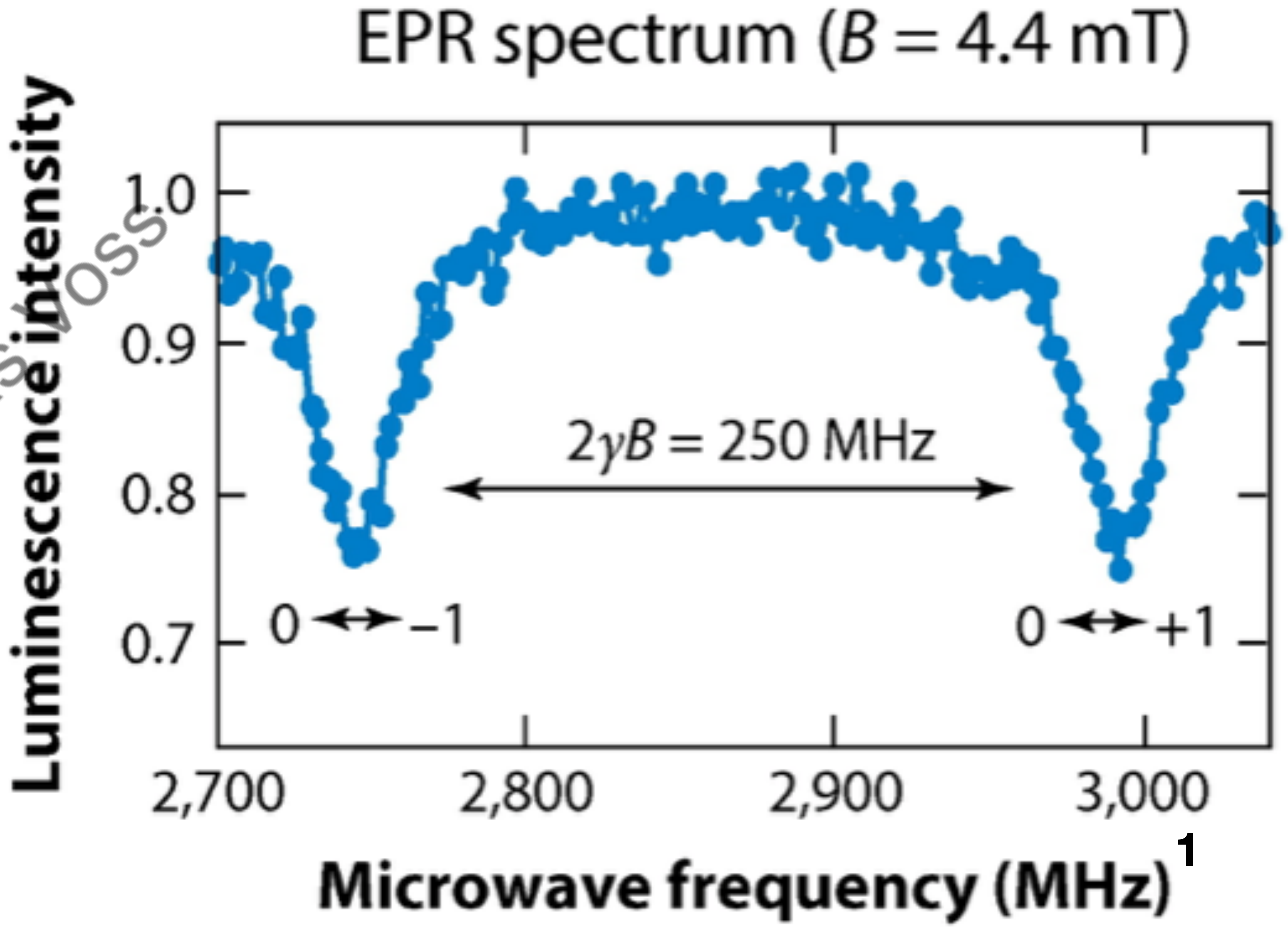
→ potential for quantum sensing

1 Herbschleb et al. *Ultra-long coherence times amongst room-temperature solid-state spins* In: Nature Communications (2019)

Motivation



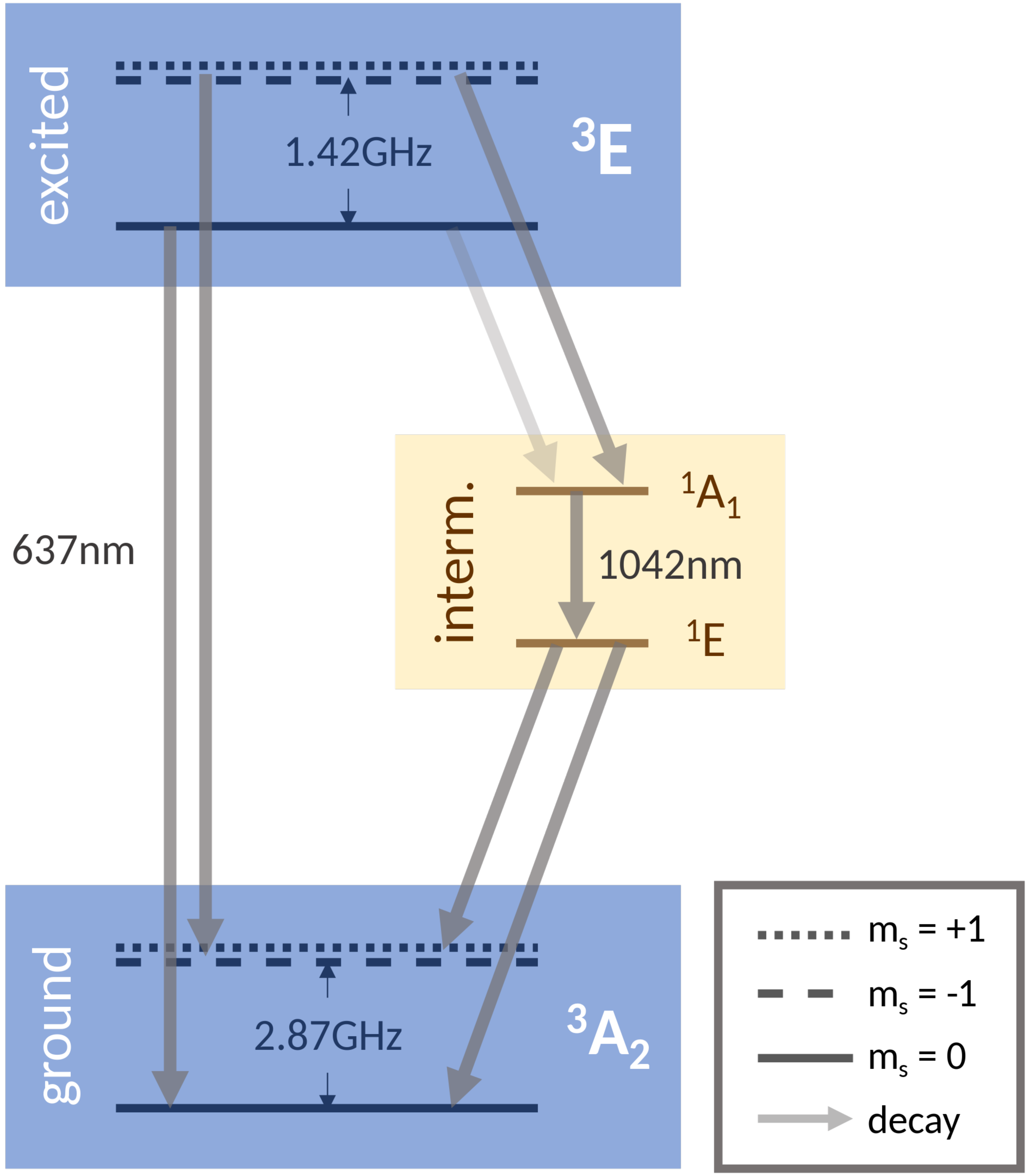
[1]



[1]

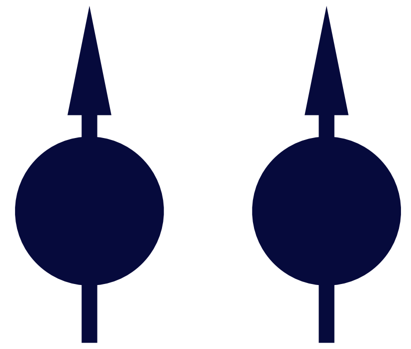
1 Romana Schirhagl et al. "Nitrogen-vacancy centers in diamond: nanoscale sensors for physics and biology". In: Annual review of physical chemistry 65 (2014), pp. 83–105

Energy level structure



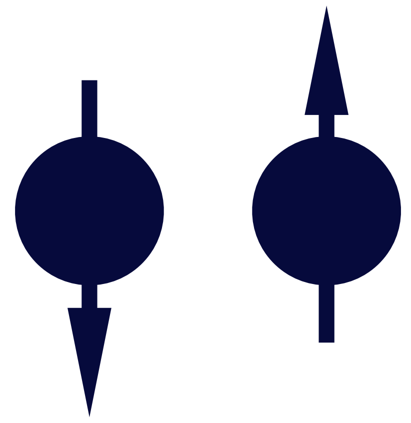
- excited-state triplet ³E

$m_s = +1$



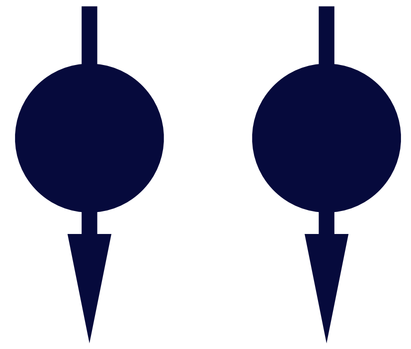
- Two intermediate-state singlets ¹A and ¹E

$m_s = 0$



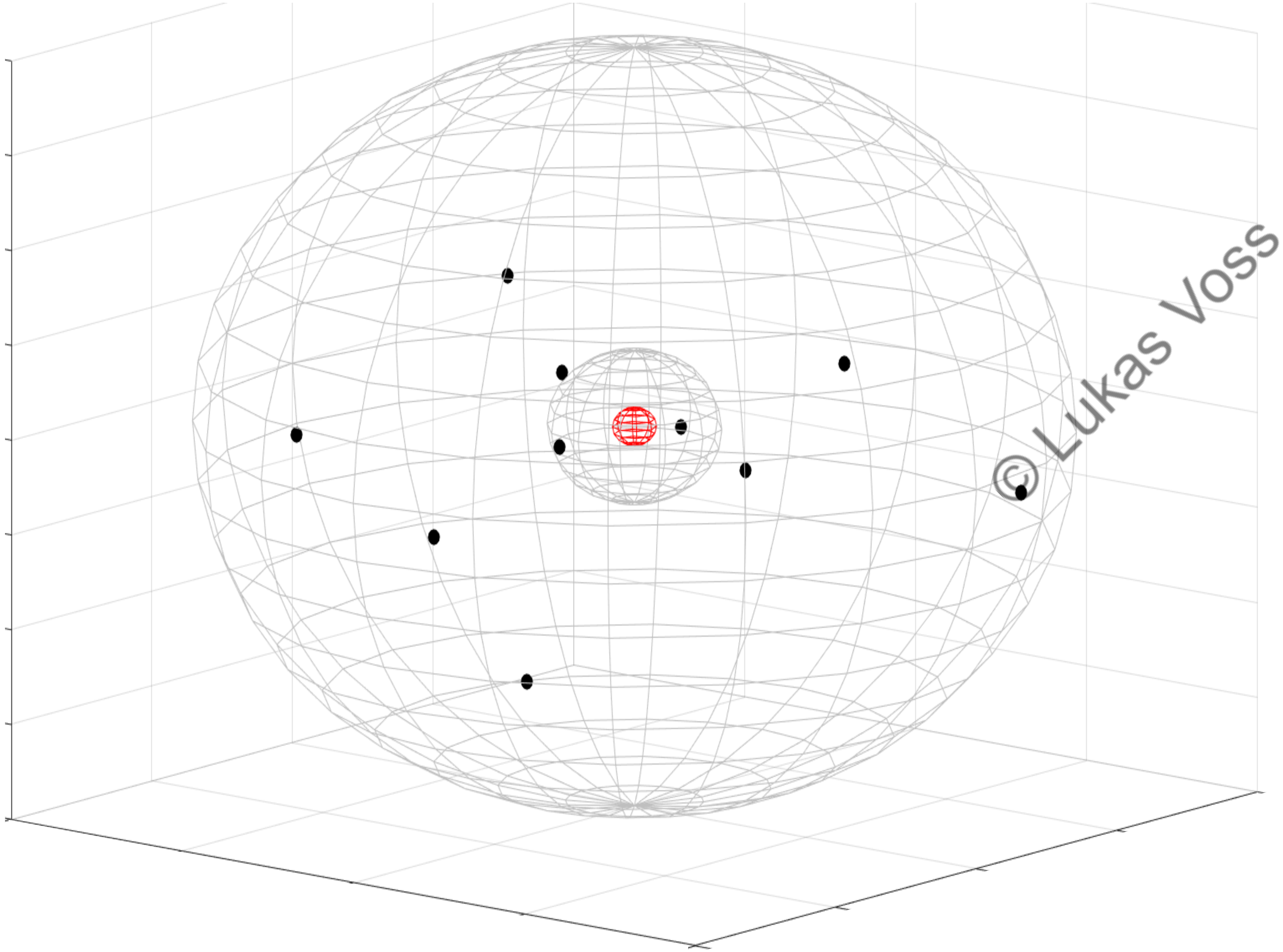
- ground-state triplet ³A

$m_s = -1$



The model

The model



- One central NV spin

$$\longrightarrow \quad S = 1$$

- Nuclear background spins of ^{13}C atoms in spherical shell

$$\longrightarrow \quad I_j = \frac{1}{2}$$

- Pairwise interaction between S and I_j

The Hamiltonian

$$H = H_{\text{NV}} + H_{\text{BS}} + H_I$$

- With the presence of a magnetic field $B = B_z$

$$H_{\text{NV}} = D\,S_z^2 + \gamma_e B_z S_z$$

$$H_{\text{BS}} = -\,\gamma_n B_z\, I_z$$

D: fine structure splitting

$\gamma_{e,n}$: gyromagnetic ratios

The Interaction Hamiltonian

$$H_I = \sum_{\alpha=1}^{N} \sum_{j \in \{x,y,z\}} \hat{S}_j \otimes \sum_{k \in \{x,y,z\}} T_{jk}^{(\alpha)} \cdot \hat{I}_k$$

- N: number of background spins
- T: dipolar tensor
- $\hat{S}$: vector of spin-1 matrices
- $\hat{I}$: vector of spin-$\frac{1}{2}$ matrices

Pairwise interaction

- Magnetic dipole-dipole interaction[1]

$$T_{KL}^{(\alpha)} = \begin{cases} \gamma_e \gamma_n \hbar^2 \left(\dfrac{3\,(R_K^{(\alpha)})^2 - (R^{(\alpha)})^2}{(R^{(\alpha)})^5} \right) & K = L \\ \gamma_e \gamma_n \hbar^2 \left(\dfrac{3\,R_K^{(\alpha)}\,R_L^{(\alpha)}}{(R^{(\alpha)})^5} \right) & K \neq L \end{cases}$$

- $\overrightarrow{R}$: connects the NV spin with nuclear spin α
- weak coupling regime due to $T_{KL}^{(\alpha)} \propto (R^{(\alpha)})^{-3}$

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1 Alexander P Nizovtsev et al. “Non-flipping 13C spins near an NV center in diamond: hyperfine and spatial characteristics by density functional theory simulation of the C510 [NV] H252 cluster”. In: New Journal of Physics 20.2 (2018)

Monte Carlo simulation

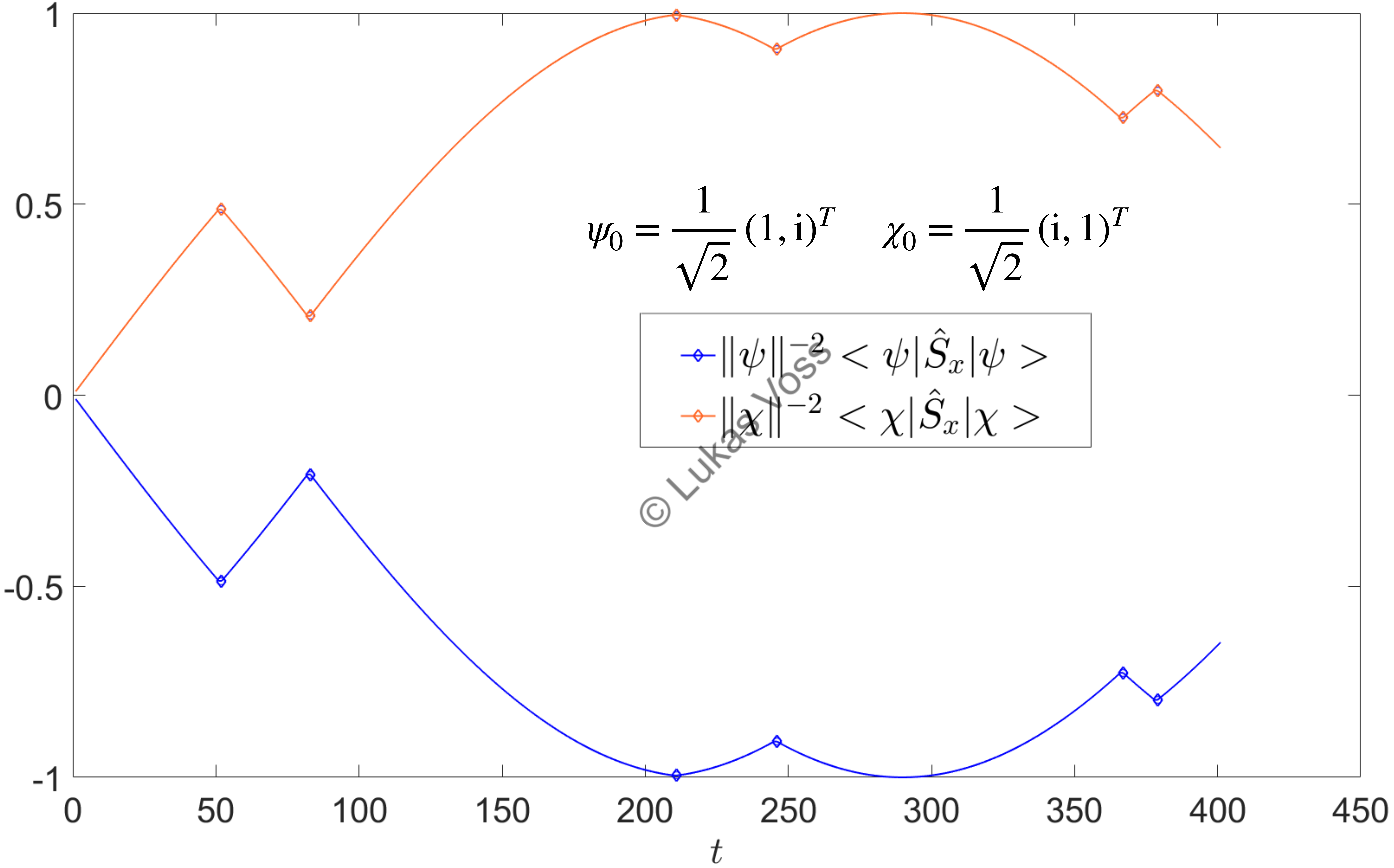
- Modified quantum jump process as proposed by Breuer[1]

$$\mathrm{d}\psi = \frac{1}{2}\Gamma\,\psi(t)\,\mathrm{d}t + \left(\sqrt{\mathrm{i}}\,\frac{\|\psi(t)\|}{\|A\,\psi(t)\|}\,A - I\right)\psi(t)\,\mathrm{d}N$$

$$\mathrm{d}\chi = \frac{1}{2}\Gamma\,\chi(t)\,\mathrm{d}t + \left(\sqrt{\mathrm{i}}\,\frac{\|\chi(t)\|}{\|B\,\chi(t)\|}\,B - I\right)\chi(t)\,\mathrm{d}N$$

→ propagate to t_{max}

1 Heinz-Peter Breuer. “Exact quantum jump approach to open systems in bosonic and spin baths”. In: Physical Review A 69.2 (2004)



1
0.5
0
-0.5
-1
0
50
100
150
200
250
300
350
400
450
t
$\psi_0 = \frac{1}{\sqrt{2}}(1, \mathrm{i})^T$
$\chi_0 = \frac{1}{\sqrt{2}}(\mathrm{i}, 1)^T$
$\|\psi\|^{-2} < \psi|\hat{S}_x|\psi >$
$\|\chi\|^{-2} < \chi|\hat{S}_x|\chi >$
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Monte Carlo simulation

Idea: Propagate states not the density matrix

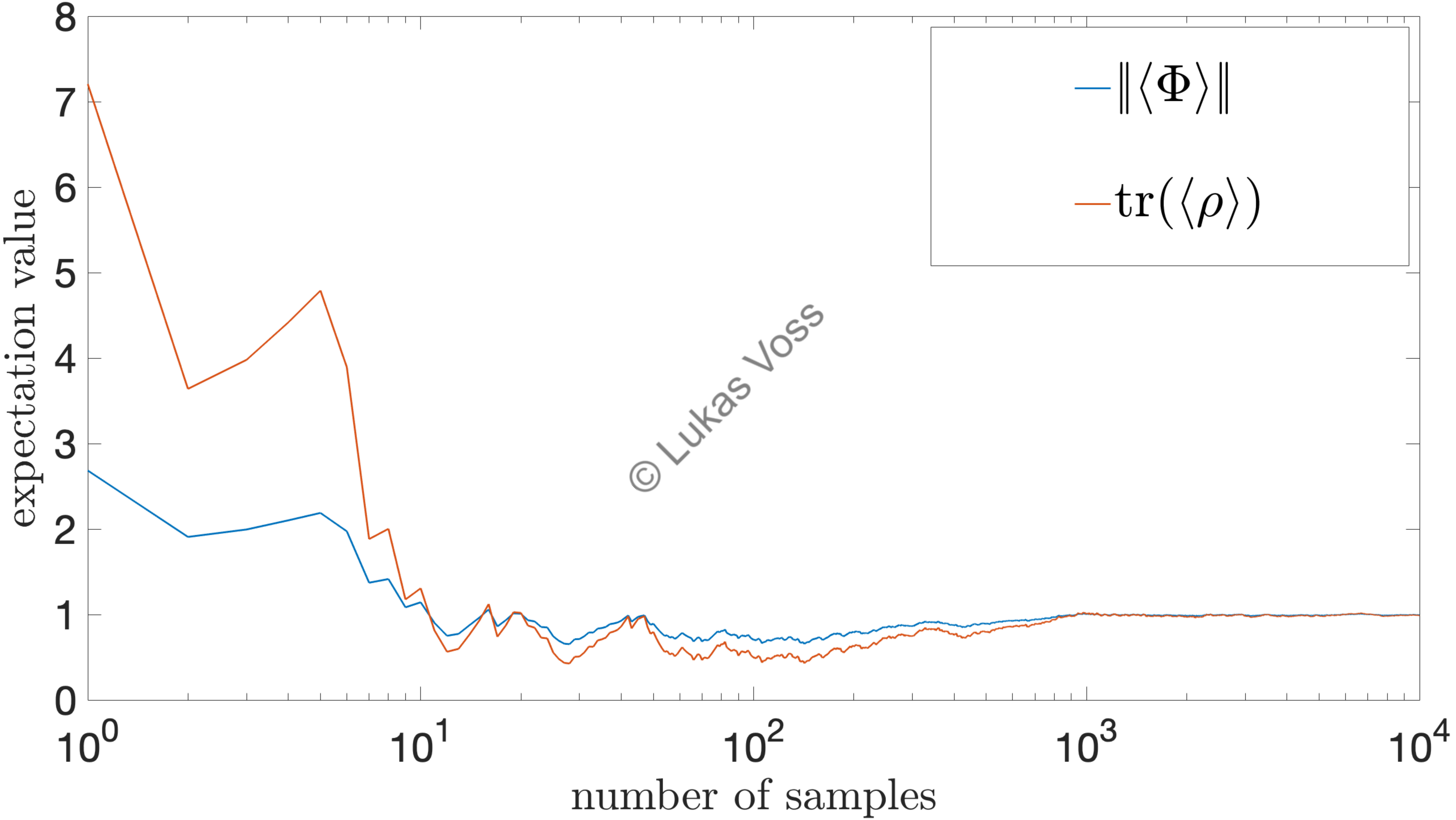
→ product state $\Phi = \psi \otimes \chi$

- The density matrix as the expectation value

$$\varrho = \mathbb{E}\big[|\Phi\rangle\langle\Phi|\big]$$

- $\mathrm{d}N$ is a differential of a Poisson increment for $\mathrm{d}t \to 0$

→ Waiting time τ between jumps is exponentially distributed



$\|\langle\Phi\rangle\|$
$\mathrm{tr}(\langle\rho\rangle)$
expectation value
number of samples
0
1
2
3
4
5
6
7
8
10^0
10^1
10^2
10^3
10^4
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Jumps for dipole interaction

- Operators A and B for a given spin component j

$$A_j \in \{S_x, S_y, S_z\} \qquad B_{j,\alpha} = \sum_{k\in\{x,y,z\}} T_{jk}^{(\alpha)} \cdot \hat{I}_k$$

- Modified stochastic differential equations

$$\mathrm{d}\psi = \frac{1}{2}\sum_{\alpha=1}^{N} \Gamma_\alpha\, \psi(t)\,\mathrm{d}t + \left(\sqrt{\mathrm{i}}\,\frac{\|\psi(t)\|}{\|A_j\,\psi(t)\|}\,A_j - I\right)\psi(t)\,\mathrm{d}N_j$$

$$\mathrm{d}\chi_\alpha = \frac{1}{2}\Gamma_\alpha\,\chi_\alpha(t)\,\mathrm{d}t + \left(\sqrt{\mathrm{i}}\,\frac{\|\chi_\alpha(t)\|}{\|B_{j,\alpha}\,\chi_\alpha(t)\|}\,B_{j,\alpha} - I\right)\chi_\alpha(t)\,\mathrm{d}N_{j,\alpha}$$

- Jump probability for spin α with spin component j

$$\Gamma_{j,\alpha}\,\mathrm{d}t = \frac{\|A_j\,\psi(t)\|\;\|B_{j,\alpha}\,\chi_\alpha(t)\|}{\|\psi(t)\|\;\|\chi_\alpha(t)\|}\,\mathrm{d}t$$

Mean Field Pivot

$$\delta A_j = A_j - \frac{\langle \psi | A_j | \psi \rangle}{\langle \psi | \psi \rangle} \qquad \delta B_{j,\alpha} = B_{j,\alpha} - \frac{\langle \chi_\alpha | B_{j,\alpha} | \chi_\alpha \rangle}{\langle \chi_\alpha | \chi_\alpha \rangle}$$

$$\longrightarrow \quad \Gamma = \Gamma(\delta A, \delta B)$$

- Adding correction terms

$$\mathrm{d}\psi = \frac{1}{2} \sum_{\alpha=1}^{N} \Gamma_\alpha \psi(t)\,\mathrm{d}t + \mathrm{i} \sum_{j=1}^{3} A_j \langle B_j \rangle \psi(t)\,\mathrm{d}t + \left(\sqrt{\mathrm{i}}\, \frac{\|\psi(t)\|}{\|\delta A_j \psi(t)\|} \delta A_j - I \right) \psi(t)\,\mathrm{d}N_j$$

$$\mathrm{d}\chi_\alpha = \frac{1}{2} \Gamma_\alpha \chi(t)\,\mathrm{d}t + \mathrm{i} \sum_{j=1}^{3} \langle A_j \rangle B_{j,\alpha} \chi_\alpha(t)\,\mathrm{d}t + \left(\sqrt{\mathrm{i}}\, \frac{\|\chi_\alpha(t)\|}{\|\delta B_{j,\alpha} \chi_\alpha(t)\|} \delta B_{j,\alpha} - I \right) \chi_\alpha(t)\,\mathrm{d}N_{j,\alpha}$$

The jump process algorithm

- All probabilities for a jump are stored in a vector with $3N + 1$ entries

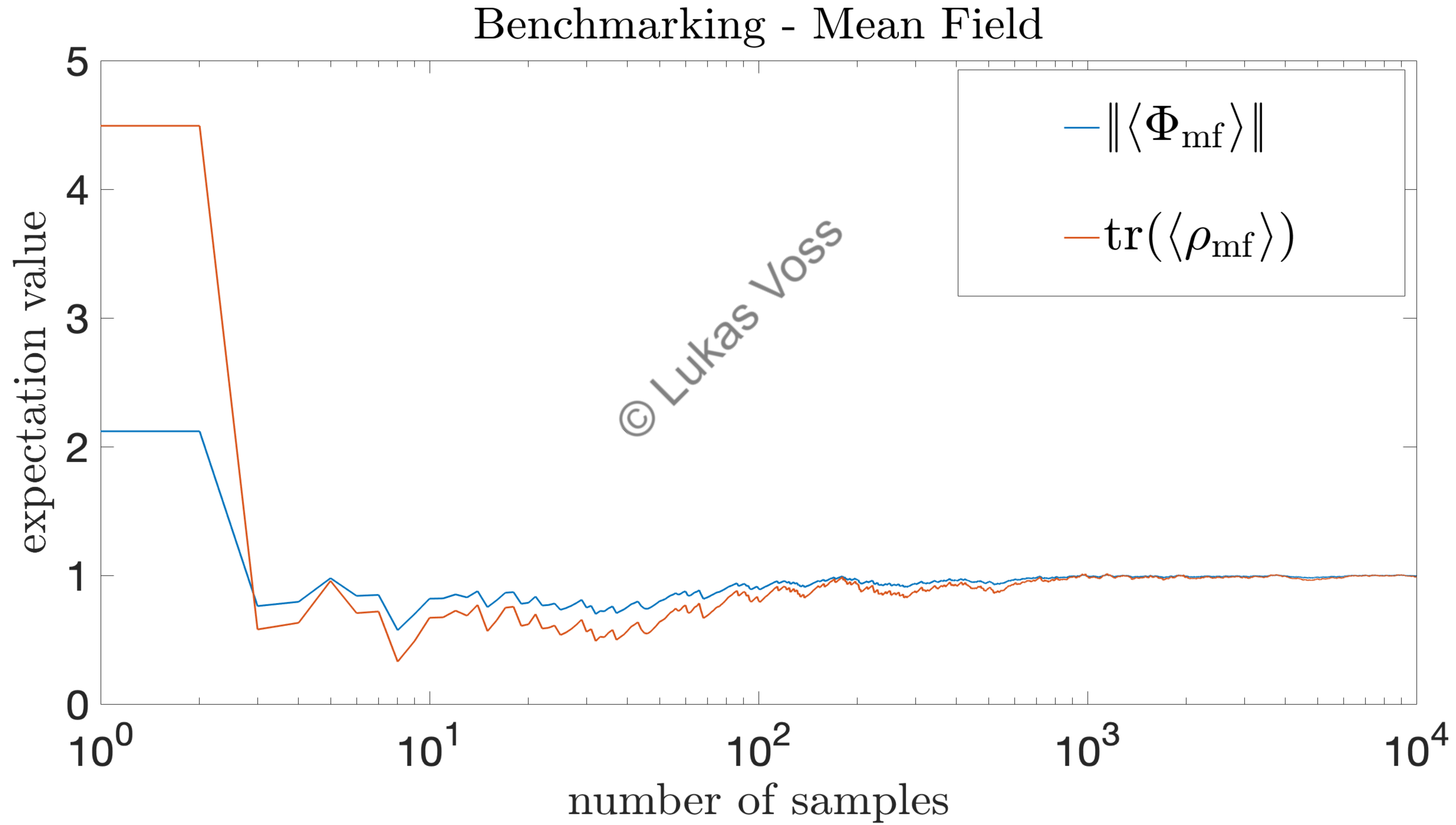
→ an index is drawn based on the probability distribution the vector forms

→ determine the background spin α and its spin component j

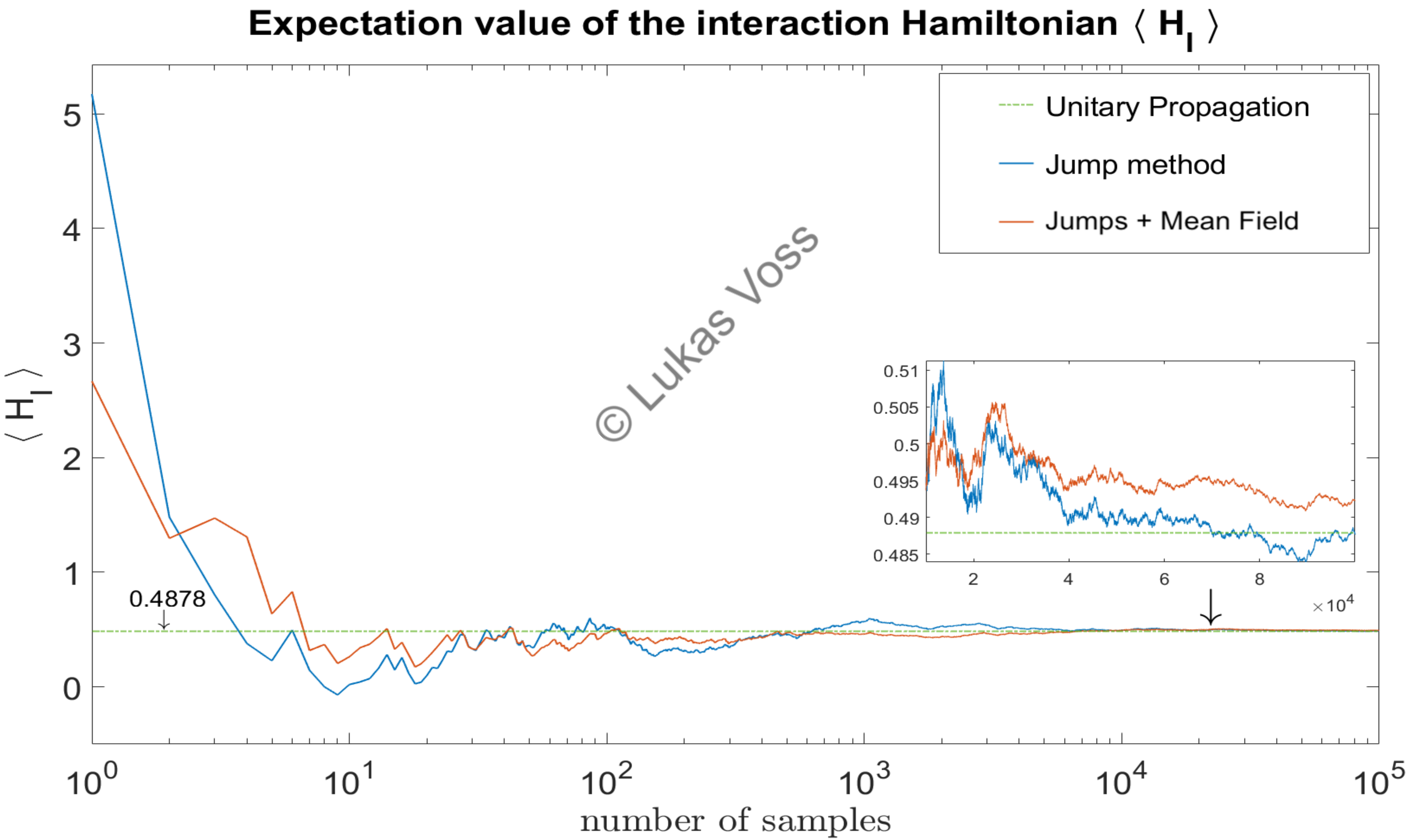
→ NV state ψ and the state of background spin χ_α perform an instantaneous jump

→ all other background spins propagate unitary and with their respective drift

Evaluation of the model



Evaluation of the model



Summary

- Effect of Mean Field is not that strong for small spins S

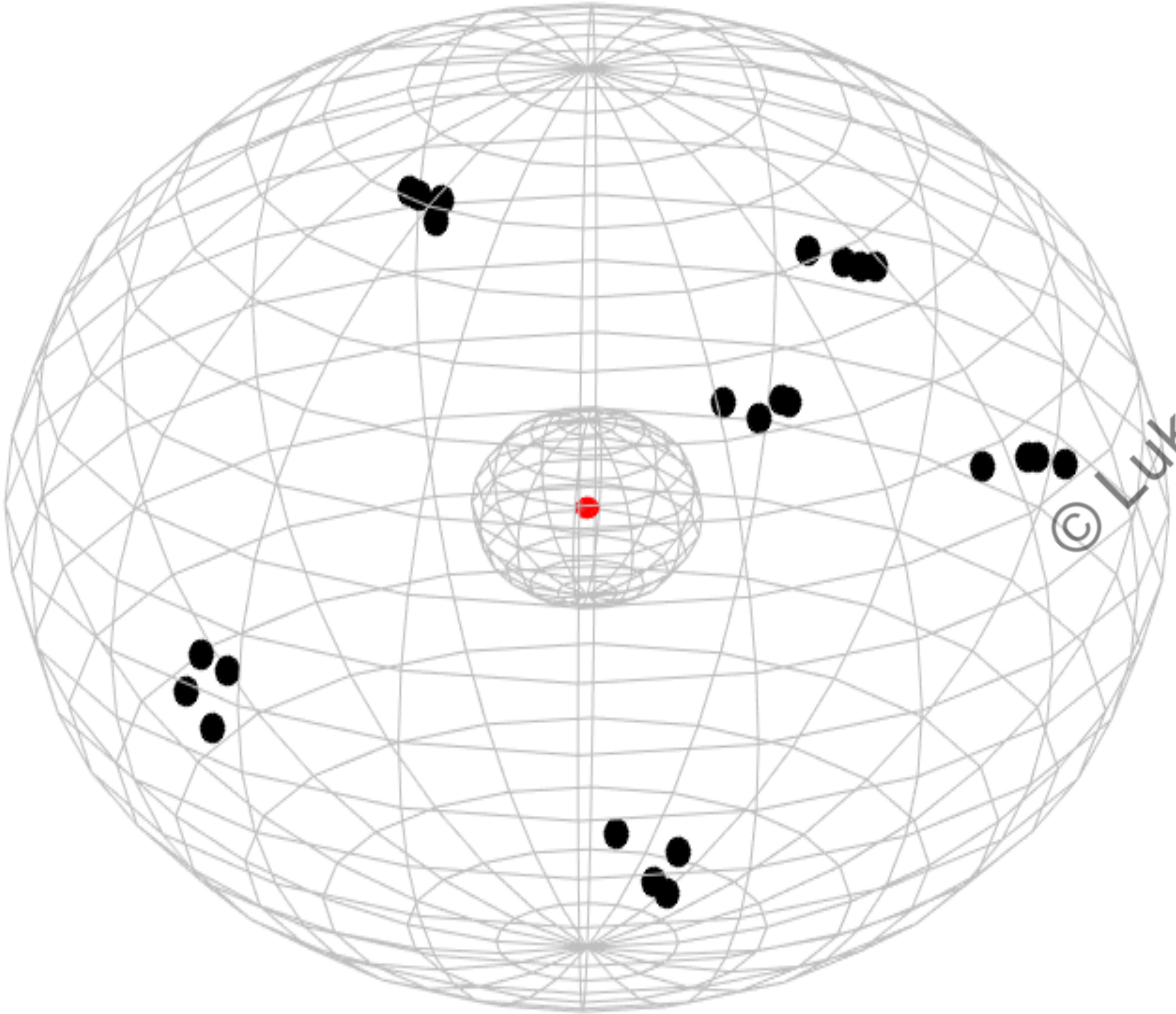
- Product state Φ remains valid for each sample

  → Overcoming the curse of dimensionality

- Number of jumps decreases for higher spins S

- Further investigation needed for more reality-based settings

Outlook and next steps



- **Clustered** nuclear background spins
- Introduce a pairwise dipolar interaction between spins within a cluster
- Pairwise interaction between clusters

Outlook and next steps

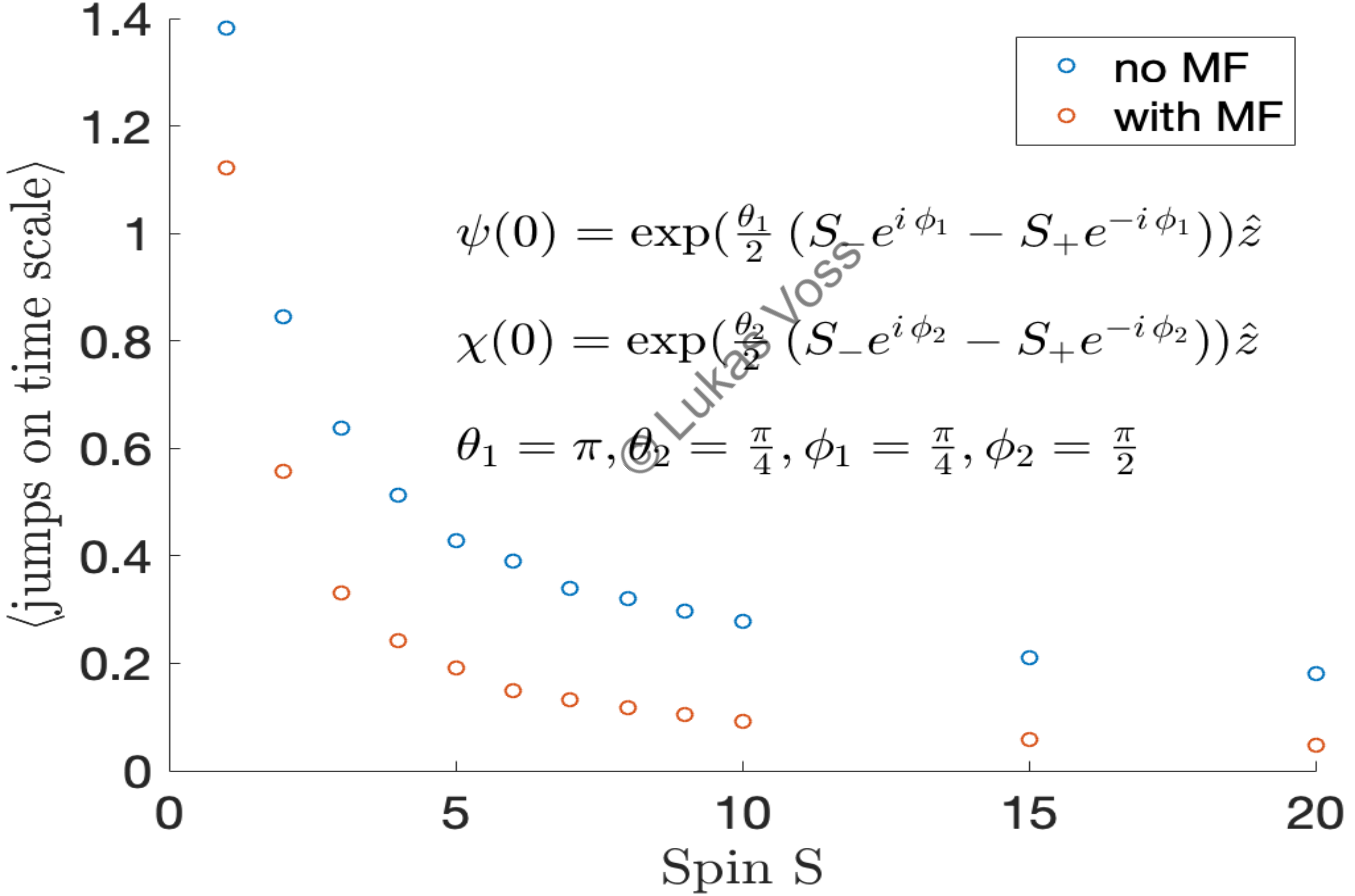
- Use a Kronecker Singular Value Decomposition (KP-SVD) for the interaction matrix

$$T^{(\alpha,\alpha')} = \sum_{j=1}^{\mathrm{rank}(T)} \tilde{\sigma}\, B_j \otimes C_j$$

→ Investigate how many singular values are necessary for a more efficient simulation

- Get in touch with Prof. Jelezko's group to get detailed information about experimental parameters to run a simulation linked to real world properties

Appendix



no MF
with MF
$\psi(0) = \exp(\frac{\theta_1}{2}\,(S_- e^{i\,\phi_1} - S_+ e^{-i\,\phi_1}))\hat{z}$
$\chi(0) = \exp(\frac{\theta_2}{2}\,(S_- e^{i\,\phi_2} - S_+ e^{-i\,\phi_2}))\hat{z}$
$\theta_1 = \pi, \theta_2 = \frac{\pi}{4}, \phi_1 = \frac{\pi}{4}, \phi_2 = \frac{\pi}{2}$
⟨jumps on time scale⟩
Spin S
0
0.2
0.4
0.6
0.8
1
1.2
1.4
0
5
10
15
20