arXiv:1311.1979

Ultra long spin decoherence times in graphene quantum dots with a small number of nuclear spins

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Journal Club, 19 November 2013

Motivation

Good qubit: long decoherence times & short operating times

$$T_2 \gg T_{op}$$

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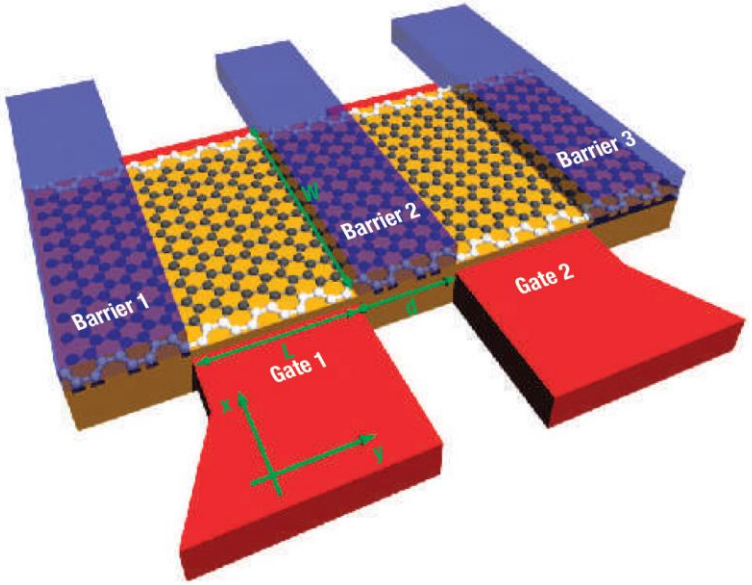
Spin qubits in graphene:



B. Trauzettel, D. V. Bulaev, D. Loss, and G. Burkard, Nature Phys. **3**, 192 (2007)

- Weak spin-orbit interaction (SOI)

  T_1 ~ milliseconds to seconds

  Struck/Burkard, PRB **82**, 125401 (2010)
  Droth/Burkard, PRB **84**, 155404 (2011)
  Droth/Burkard, PRB **87**, 205432 (2013)
  Hachiya/Burkard/Egues, arXiv:1307.4668

- Weak hyperfine interaction

  Fischer/Trauzettel/Loss, PRB **80**, 155401 (2009)

Motivation

Previous work by the authors:

Fuchs/Rychkov/Trauzettel, Phys. Rev. B **86**, 085301 (2012)

Electron spin decay in a **nuclear spin bath**,
in the presence of large external magnetic fields

→ Generalized master equation (Nakajima-Zwanzig),
see also Coish/Fischer/Loss

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Electron spin decay in a **nuclear spin bath**,
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→ Generalized master equation (Nakajima-Zwanzig),
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Here:

Graphene quantum dots with **less than 10 nuclear spins**

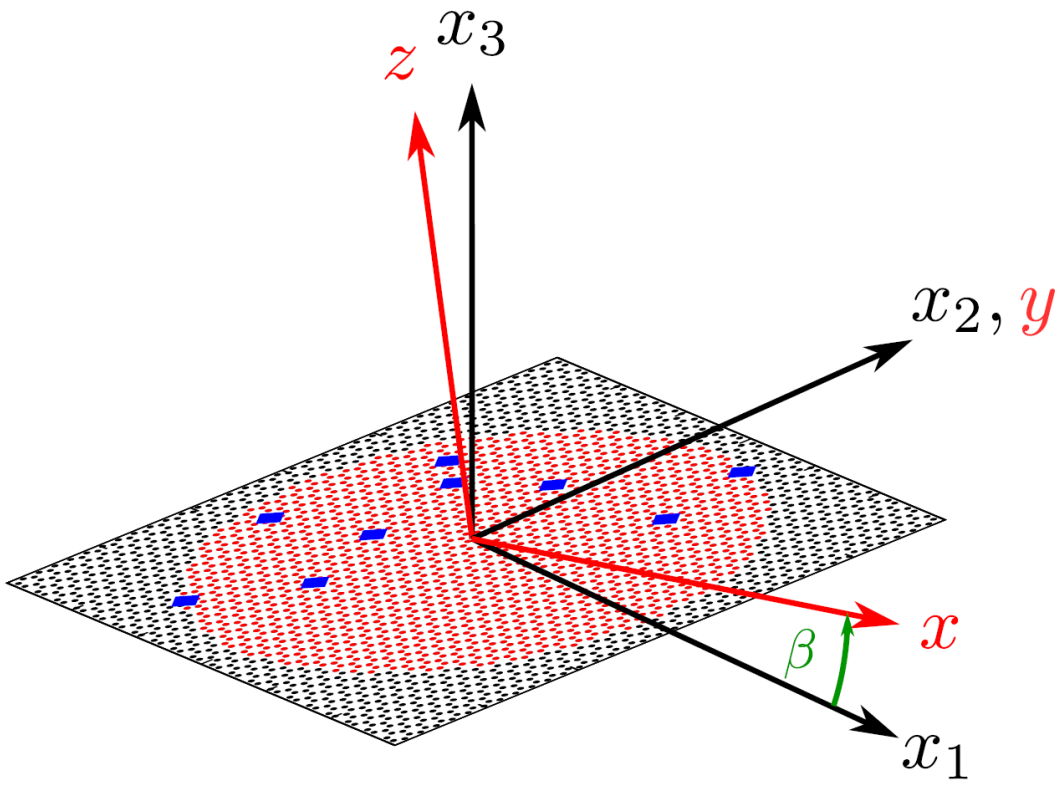
→ Positions and initial states can be very important

Schliemann/Khaetskii/Loss, Phys. Rev. B **66**, 245303 (2002)
Schliemann/Khaetskii/Loss, J. Phys.: Condens. Matter **15**, R1809 (2003)

Model: Coordinate Systems

z axis: - spin quantization axis

- direction of external magnetic field (for initialization)



$\beta = 0$: $z \perp$ graphene sheet

$\beta = \pi/2$: $z \parallel$ graphene sheet

Model: Quantum Dot

Gaussian envelope function: $\phi(\vec{r}) = \phi_0 \exp\left[-\frac{1}{2}\left(\frac{r}{R}\right)^2\right] = \phi(r) \qquad r = |\vec{r}|$

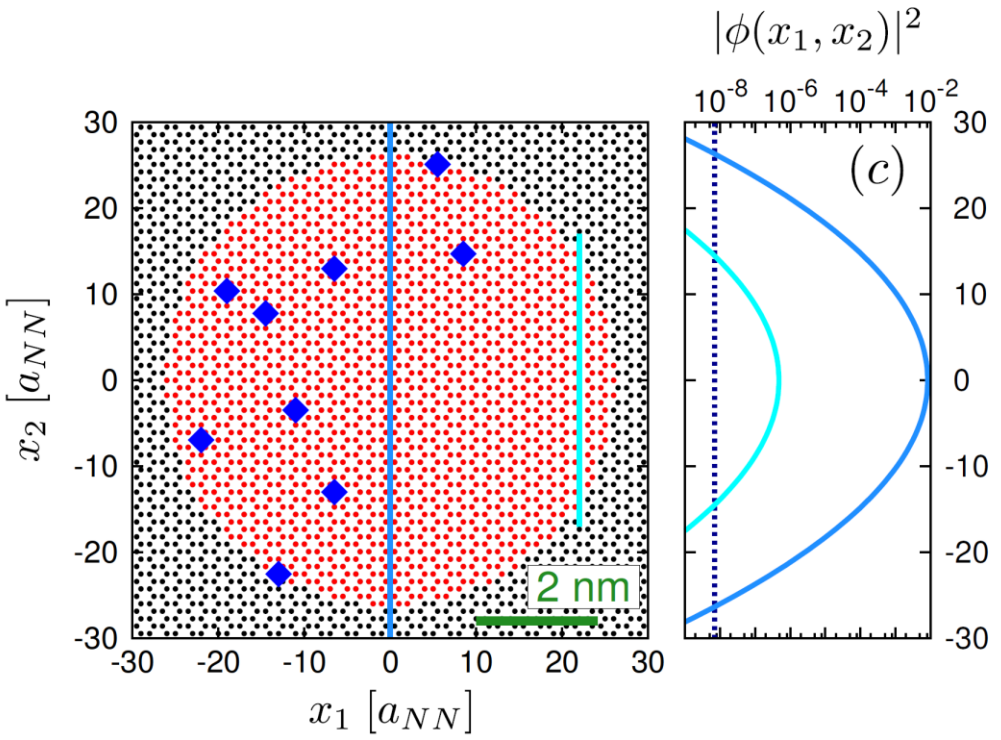
same function for both sublattices

The QD consists of N_{sites} lattice sites at positions $\{\vec{r}_k\}_{i=1}^{N_{sites}}$, where

$$\frac{|\phi(\vec{r}_i)|^2}{|\phi(\vec{r}_{max})|^2} > C$$

Cut-off: $C = 10^{-6}$

Normalization: $\sum_{i=1}^{N_{sites}} |\phi(\vec{r}_i)|^2 = 1$



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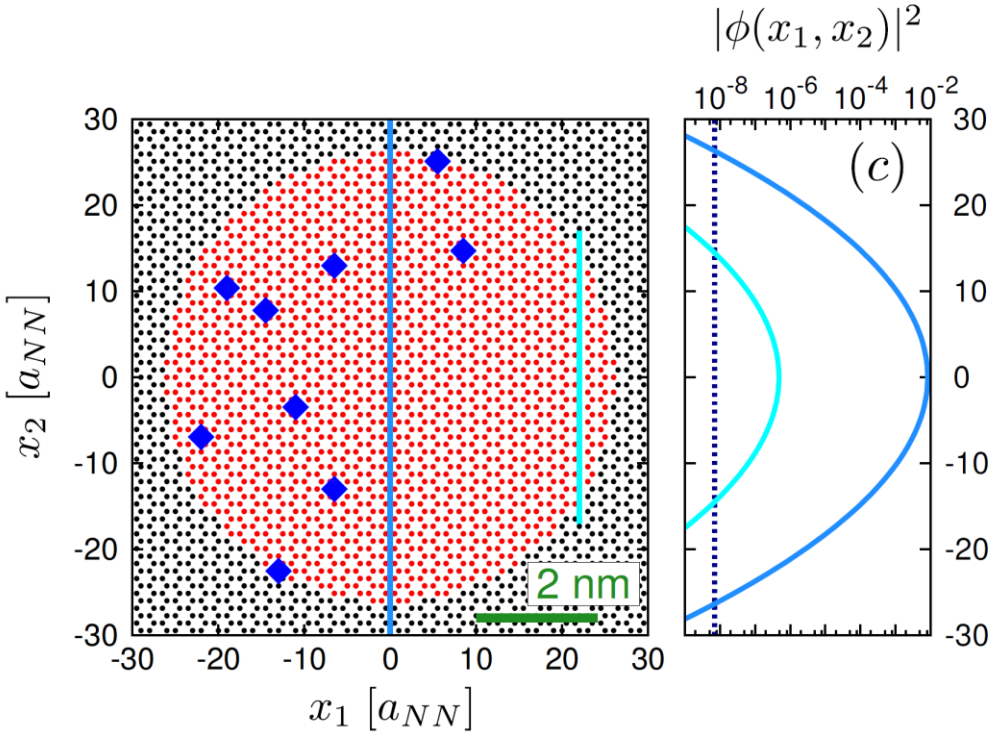
Simulations:

R ≈ 3.6 nm, $N_{sites} \approx 10^3$

K nuclear spins at random positions, with equal probability for each lattice site in the QD

$$2 \le K \le 9$$

$K \sim 9$:
natural abundance of ^{13}C in carbon



Model: Hamiltonian

Hyperfine interaction: $\hat{H}_{HI} = A_{HI} \sum_{k=1}^{K} \sum_{\mu,\nu} \overleftrightarrow{A}_{\mu\nu} |\phi(\vec{r}_k)|^2 \hat{S}_\mu \hat{I}_{k,\nu}$

In graphene coordinate system:

$$\overleftrightarrow{A} = \begin{pmatrix} -\frac{1}{2} & 0 & 0 \\ 0 & -\frac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$A_{HI} = 0.6\,\mu\mathrm{eV}$

2nd rank tensor

electron spin

nuclear spin

Fischer/Trauzettel/Loss, PRB **80**, 155401 (2009)

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Zeeman energy: $\hat{H}_{ZE} = \hbar\gamma_S B_z \hat{S}_z + \hbar\gamma_{13C} B_z \sum_{k=1}^{K} \hat{I}_{k,z} \approx A_{ZE} \hat{S}_z$

neglected because of the small gyromagnetic ratio

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No direct coupling among nuclear spins

No spin-orbit interaction

Time Evolution & Exact Diagonalization

Time-dependent expectation value of an operator *O*:

$$\langle O \rangle(t) = \langle \psi_0 |\ \hat{U}^{\dagger}(t)\, \hat{O}\, \hat{U}(t)\ | \psi_0 \rangle$$

$$\hat{U}(t)\ =\ \exp[-\mathrm{i}\hbar^{-1} t\, \hat{H}]$$

initial state, electron spin and nuclear spins

$H = H_{HI} + H_{ZE}$: total Hamiltonian

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Basis states:

$$|n\rangle = |m_S^n\rangle \otimes \bigotimes_{k=1}^{K} |m_k^n\rangle = |\Downarrow\uparrow\downarrow\downarrow\uparrow \ldots\rangle$$

electron spin nuclear spins

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electron spin nuclear spins

For $K < 10$ considered here, the time evolution can be calculated numerically via a unitary matrix *M* that diagonalizes *H.*

This matrix *M* is found using the EIGEN package for C++.

Simulation

At time $t = 0$, the electron spin is considered in the "down" state:

$|\psi_0\rangle$ is a linear combination of states $|\Downarrow \ldots\rangle$

quantization along z axis

complex coefficients chosen randomly

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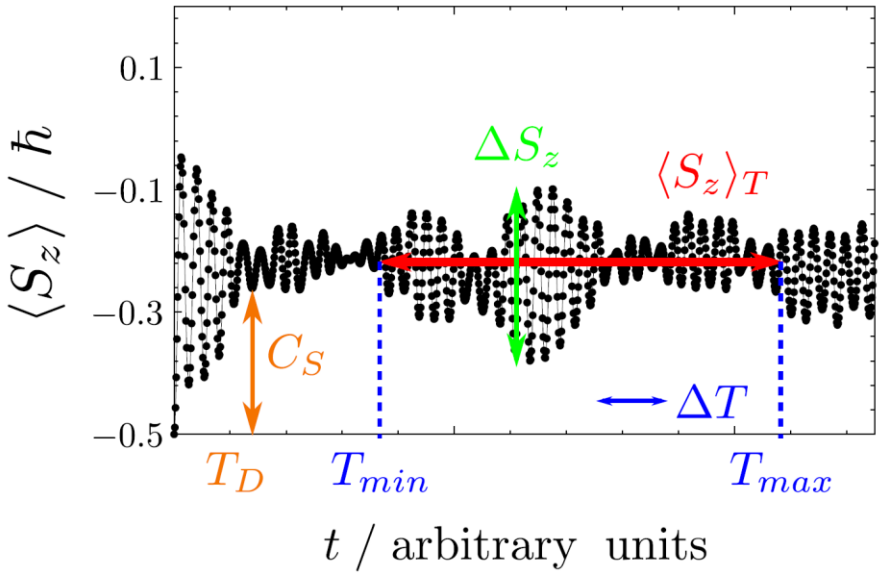
Basis for all results discussed in the following:

At **zero external magnetic field**, calculate the **expectation value of the longitudinal electron spin component** $\langle S_z \rangle(t)$ for t > 0



example for given configuration and initial state of the nuclear spins

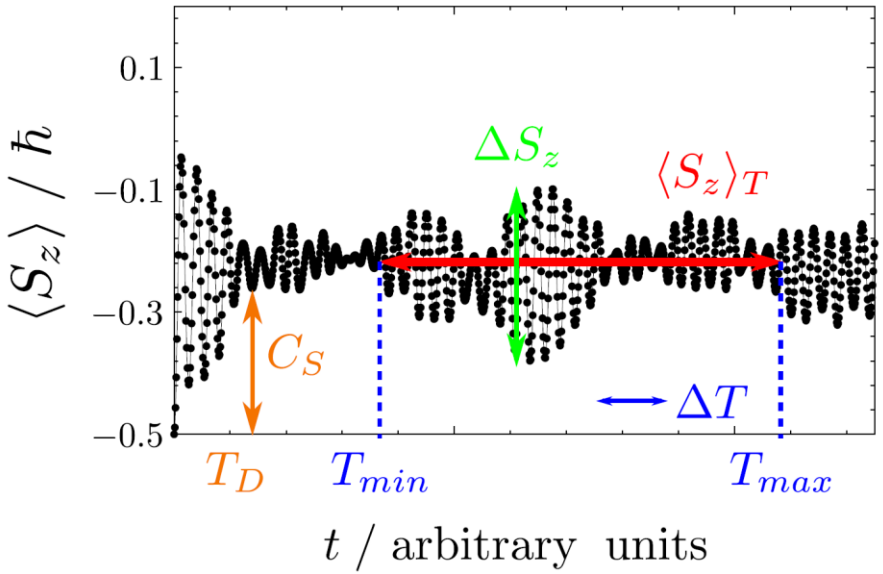
Longtime Average

Longtime average: $$\langle S_z \rangle_T = \frac{1}{N_T} \sum_{s=0}^{N_T} \langle S_z \rangle (T_{min} + s \cdot \Delta T)$$

"We found stable values for:"

$$T_{min} = 0.5 \times 10^9 \tau_{HI}$$
$$T_{max} = 1.5 \times 10^9 \tau_{HI}$$
$$\Delta T = 10^4 \tau_{HI}$$

$$\tau_{HI} = \hbar / A_{HI} \approx 1\,\mathrm{ns}$$



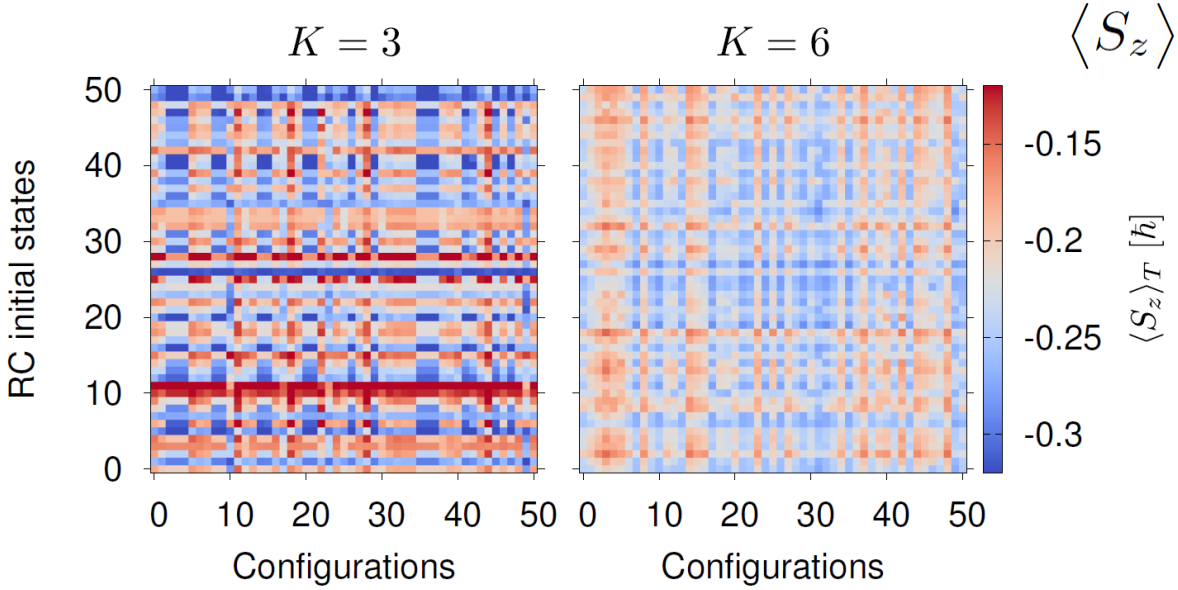
example for given configuration and initial state of the nuclear spins

Longtime Average: $\beta = 0$

Longtime average for out-of-plane case:

average over all 51x51 *initial conditions:*

$$\langle S_z \rangle_T \approx -0.22\,\hbar$$



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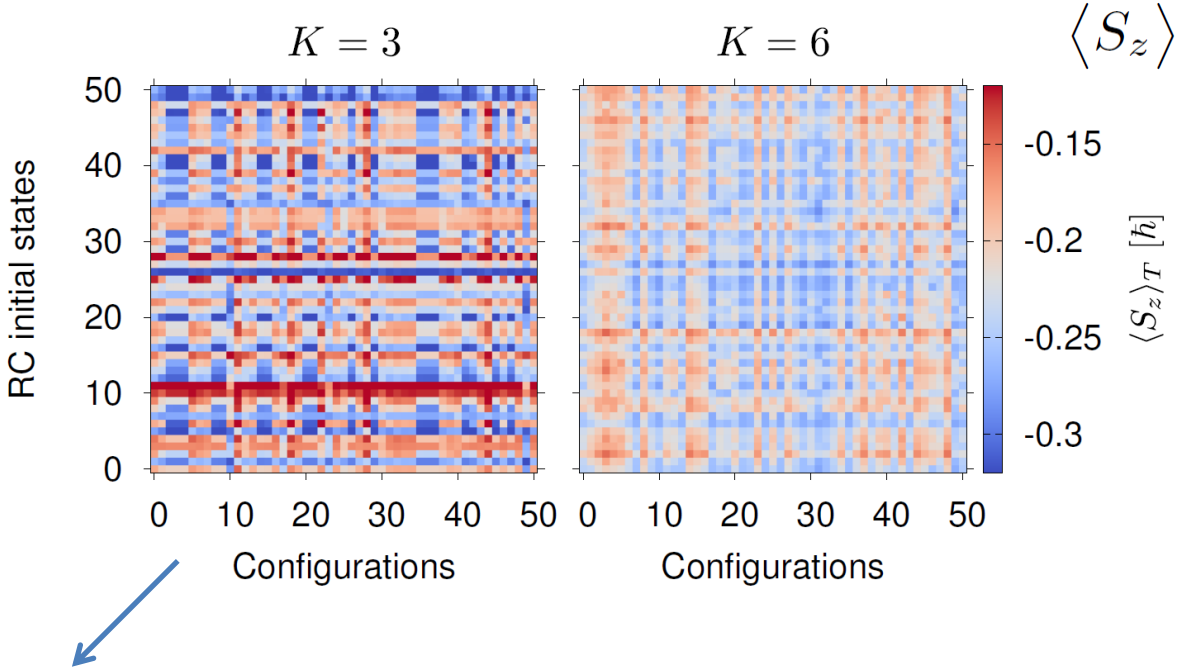

- Weak dependence on positions
- Strong dependence on initial state

Explanation:
Usually, only one nuclear spin interacts strongly with the electron spin

Longtime Average: $\beta = 0$

Longtime average for out-of-plane case:

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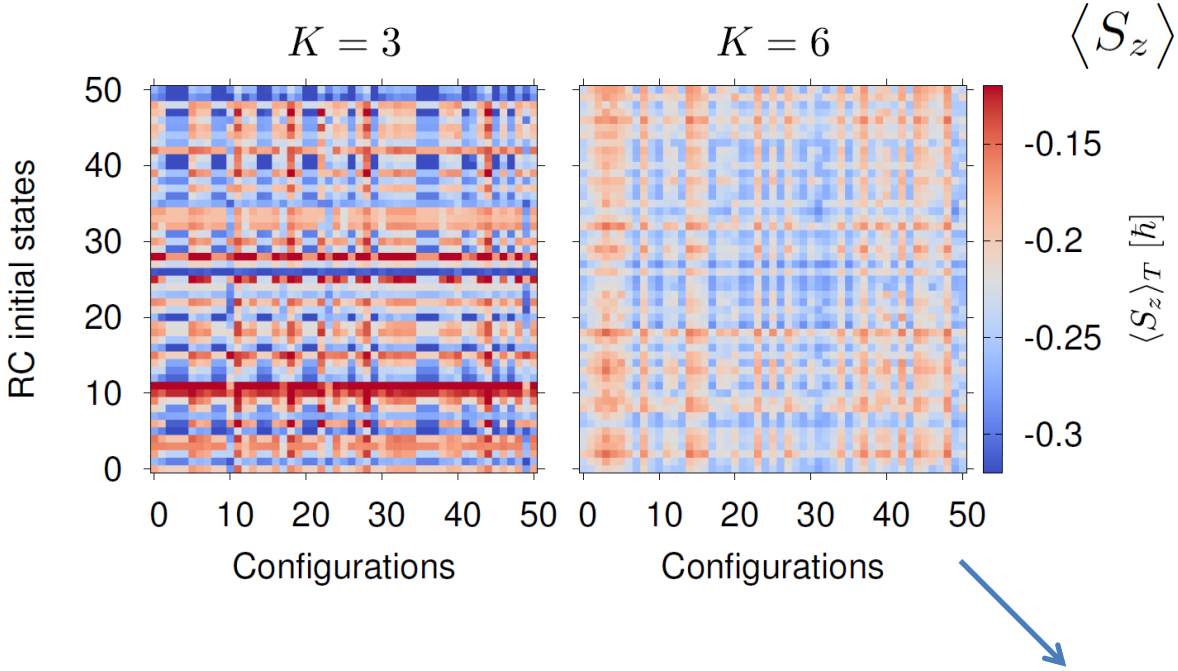
$$\langle S_z \rangle_T \approx -0.22\,\hbar$$

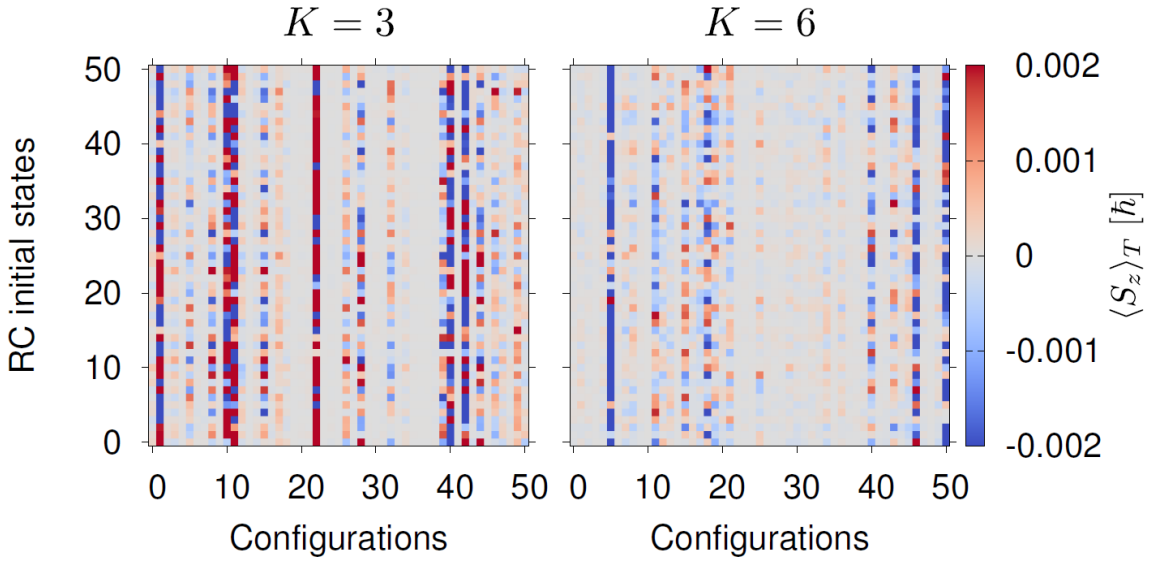


Weaker dependence on initial state

Explanation:
Larger Hilbert space results in more effective averaging

Longtime Average: $\beta = \pi/2$

Longtime average for in-plane case:



In stark contrast to $\beta = 0$, the longtime average (always) vanishes

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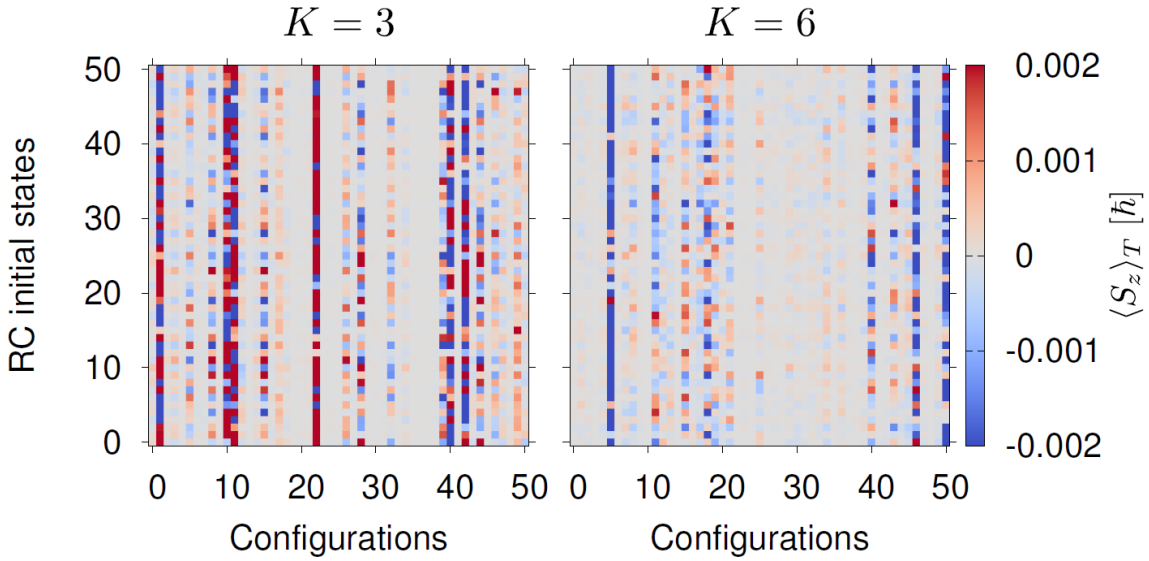
Longtime average for in-plane case:



In stark contrast to $\beta = 0$, the longtime average (always) vanishes

Explanation from analytical calculation for $K = 1$:

$$\langle S_z \rangle_T(\beta) = \lim_{\Delta T \to \infty} \frac{1}{2\Delta T} \int_{T+\Delta T}^{T-\Delta T} \langle S_z \rangle(t, \beta) =$$

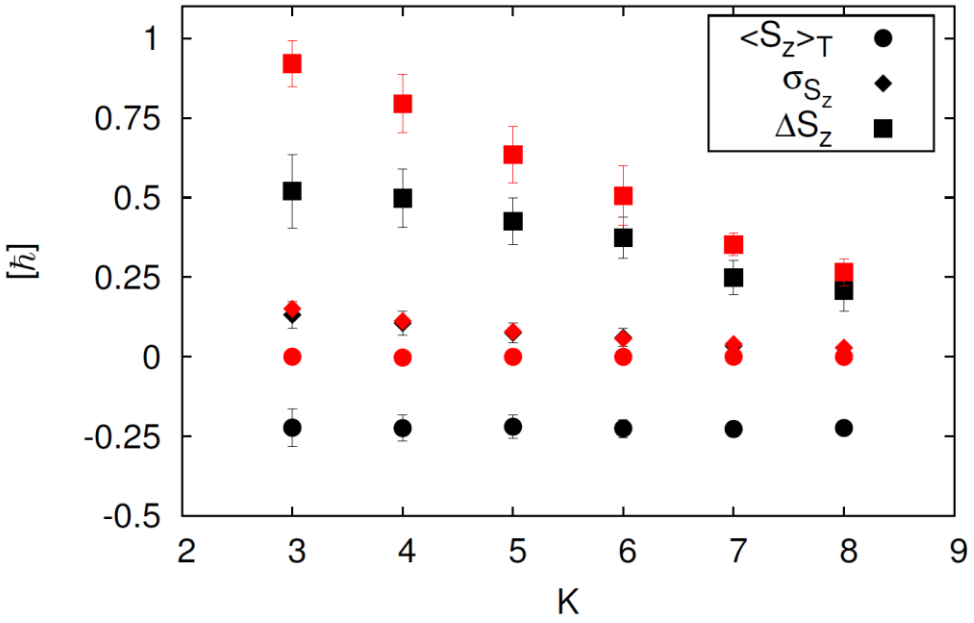
$$-\frac{\hbar}{4} \cos(\beta) \left[2\rho_{\downarrow\downarrow} \cos(\beta) + (\rho_{\uparrow\downarrow} + \rho_{\downarrow\uparrow}) \sin(\beta) \right]$$

Density matrix at t = 0

$$\rho_0 = |\psi_0\rangle \langle\psi_0| = \begin{pmatrix} \rho_{\downarrow\downarrow} & \rho_{\downarrow\uparrow} & 0 & 0 \\ \rho_{\uparrow\downarrow} & \rho_{\uparrow\uparrow} & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

Dependence on *K*

Average over all 51x51 initial conditions:

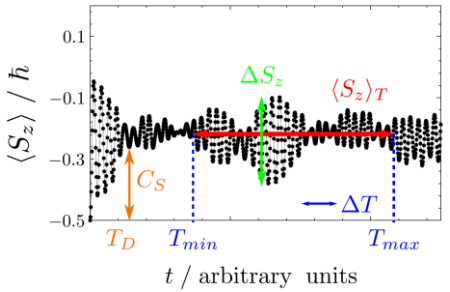


Black: $\beta = 0$

Red: $\beta = \pi/2$

Standard deviation: $$\sigma_{S_z} = \sqrt{\frac{1}{N_T}\sum_{s=0}^{N_T}\left(\langle S_z\rangle(T_{min}+s\cdot\Delta T)-\langle S_z\rangle_T\right)^2}$$

Sample range: $$\Delta S_z = \max_{T_{min},T_{max}}\left[\langle S_z\rangle(t)\right] - \min_{T_{min},T_{max}}\left[\langle S_z\rangle(t)\right]$$

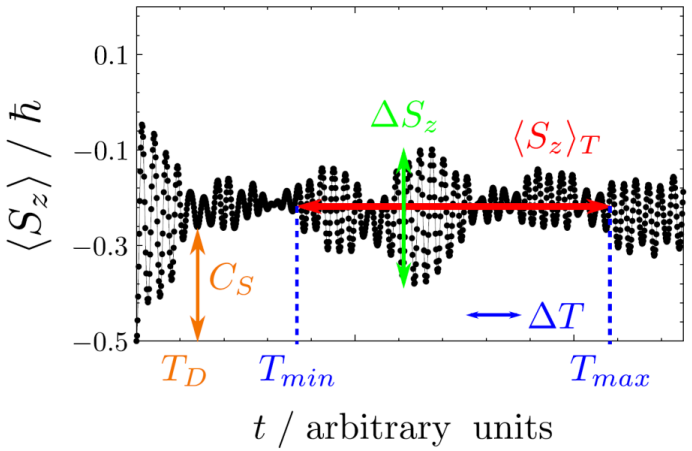


Standard deviation and sample range decrease with increasing *K*

Decoherence Time

Definition of the decoherence time T_D:

Time after which the oscillation amplitude decreased below the threshold value C_S



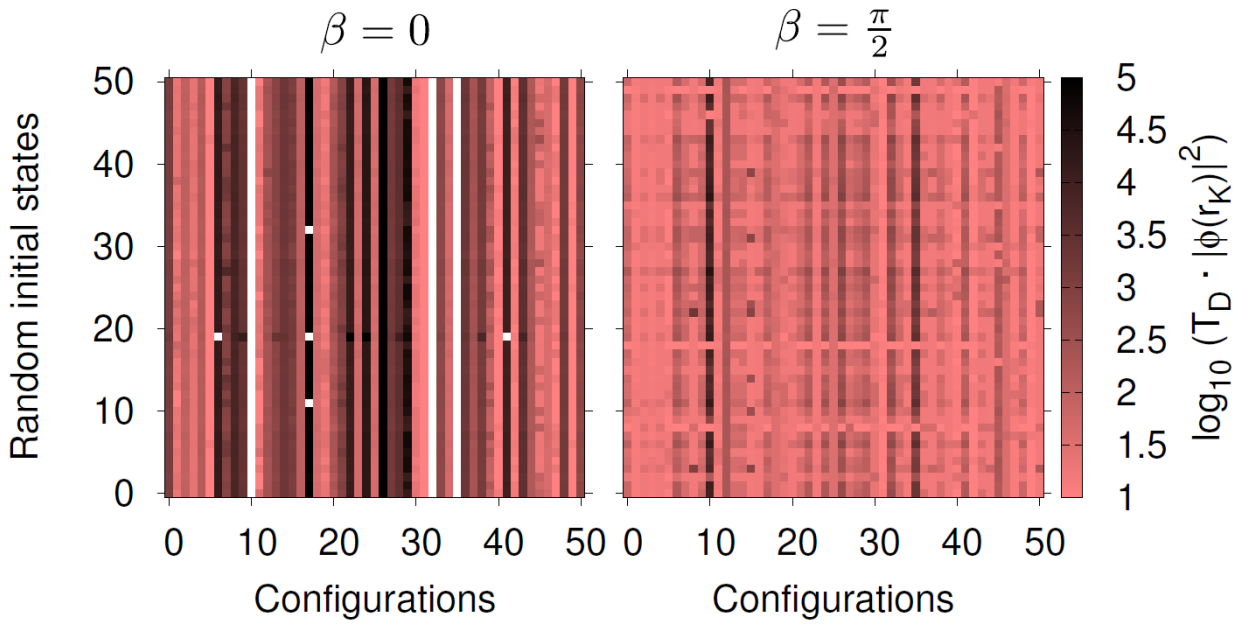
Out-of-plane case $\beta = 0$: $C_S = -0.325\,\hbar$

In-plane case $\beta = \pi/2$: $C_S = -0.1\,\hbar$

Decoherence Time

Results for $K = 6$:

renormalized by electron probability at the nuclear spin with strongest coupling



white:
no decoherence before 0.1 s

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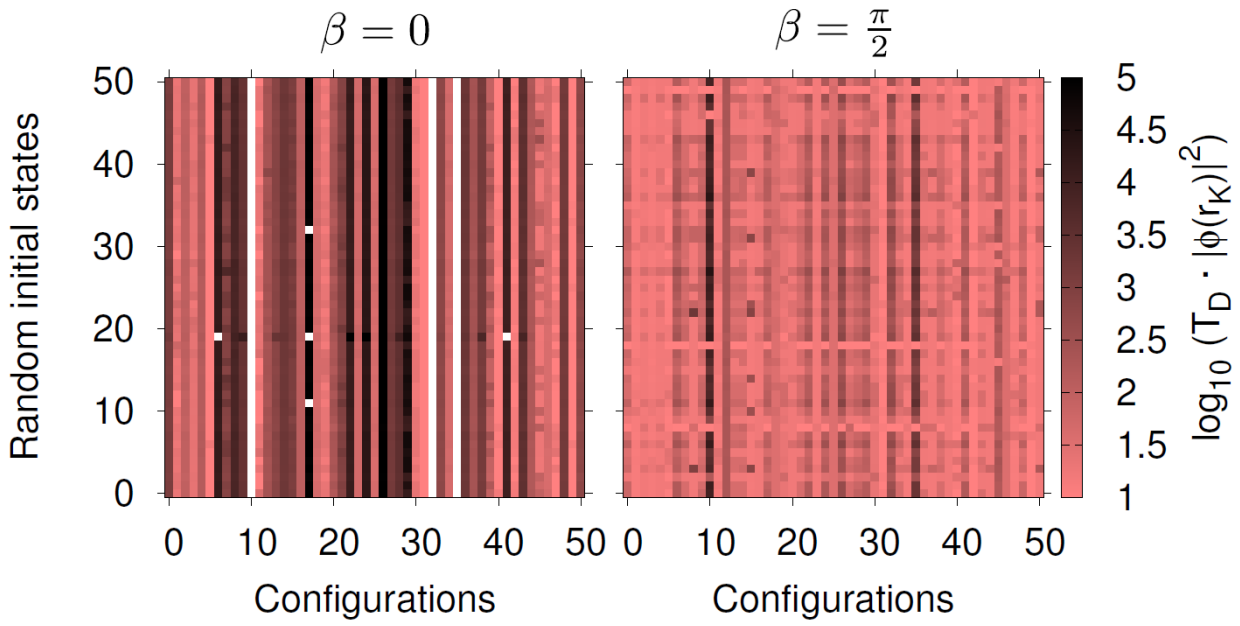


white:
no decoherence
before 0.1 s

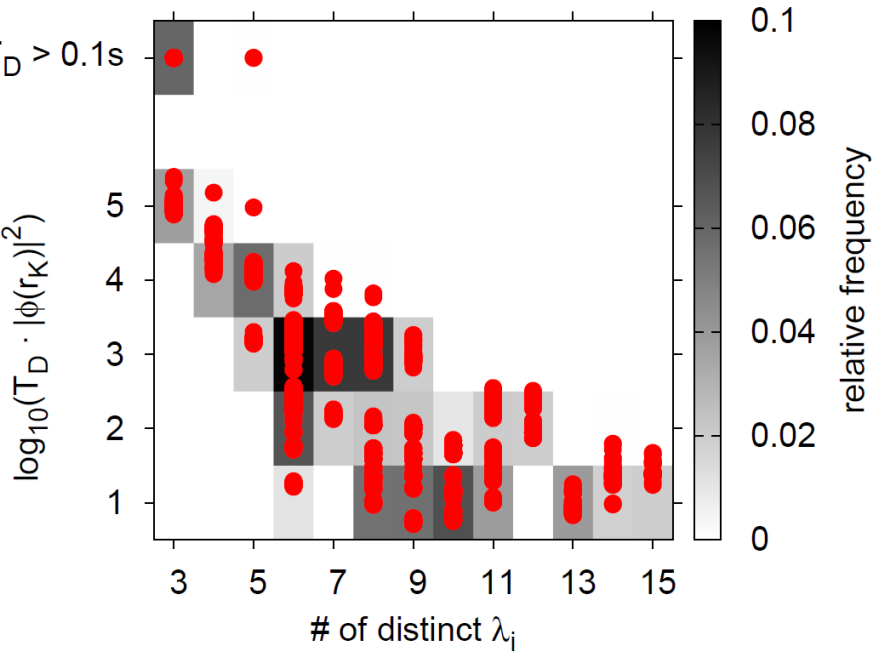
- weak dependence on initial state
- **very strong dependence on nuclear spin positions**

Decoherence Time: $\beta = 0$

Correlation to number of distinct eigenvalues:

$K = 6$

$\beta = 0$



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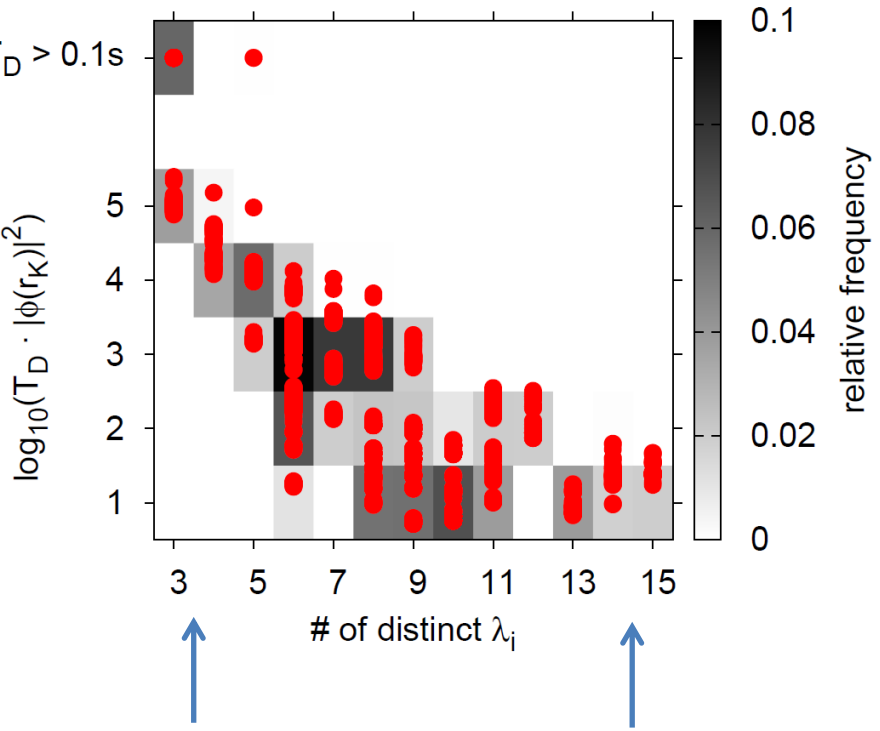


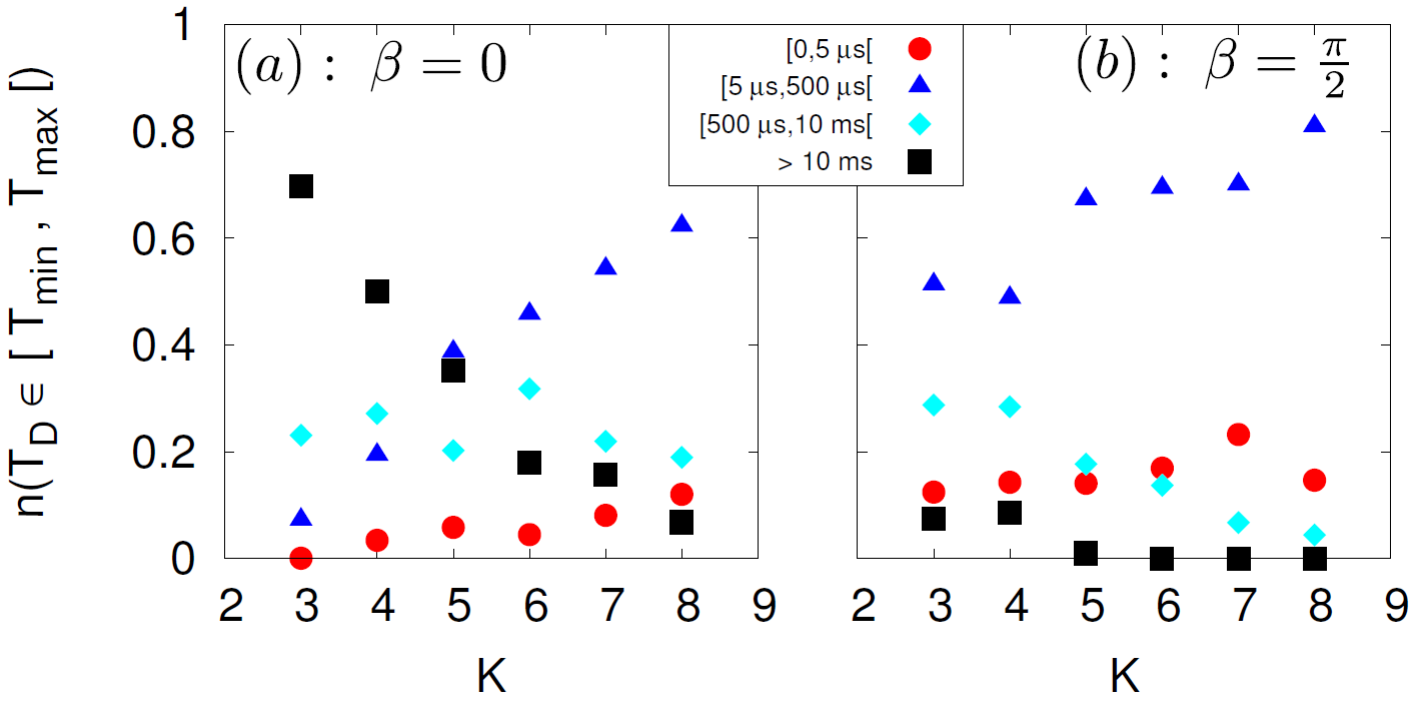
only **one** nuclear spin interacts strongly with the electron spin

several nuclear spins are equally coupled to the electron spin

In combination with the form of the hyperfine interaction tensor, this leads to the observed results

Decoherence Time

Absolute value of the decoherence time:



Particularly long T_D in the out-of-plane case ($\beta = 0$) at small K

T_D is quite long in general, on the order of hundreds of microseconds

Conclusions

- Long decoherence times T_D were found for graphene QDs with very few nuclear spins

  Interesting questions, among others:
  What is the outcome when $\langle \boldsymbol{S} \rangle(t)$ is averaged over the initial states?
  What will be the lifetimes in the presence of a magnetic field?

- Even longer decoherence times may be achieved using echo pulses

- In graphene QDs with very few nuclear spins, other decay channels can dominate

  E.g., phonon-mediated relaxation times down to $\sim$ 1 ms were predicted

  Struck/Burkard, PRB **82**, 125401 (2010); Droth/Burkard, PRB **84**, 155404 (2011);
  Droth/Burkard, PRB **87**, 205432 (2013); Hachiya/Burkard/Egues, arXiv:1307.4668

- Graphene quantum dots are promising platforms for quantum information processing