Dekoherencia és összefonódottság csatolt nanomágnes gyűrűkben

Szállás Attila

"Félvezető nanoszerkezetek" kutatócsoport
Elméleti Szilárdtestfizikai Osztály
MTA Wigner Fizikai Kutatóközpont

Entanglement Day

2014. szept. 5.-6.

Collaborators

Collaborators:

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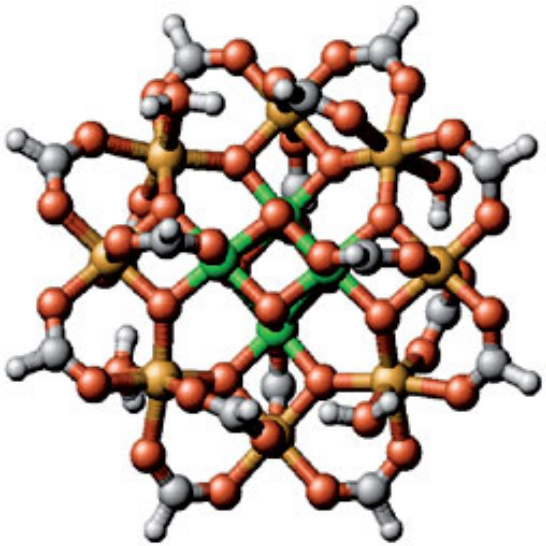
Funding:

CNR, Università degli Studi di Modena e Reggio Emilia

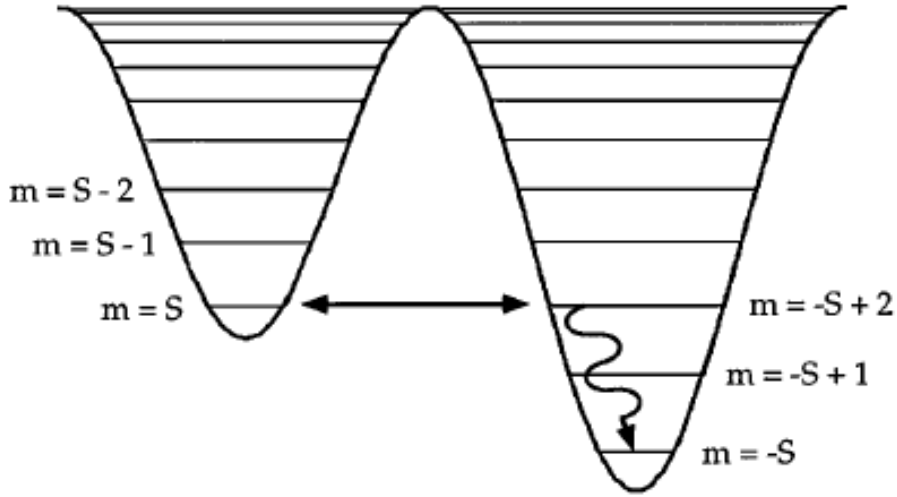
Quantum tunneling of the magnetization

Mn_{12} (S=10)



"Giant spin" model

$$H = -DS_z^2 + g\mu_B S_z$$



large spin and large easy-axis anisotropy $\Longrightarrow$ bistable system with slow relaxation of magnetization, limited by quantum tunneling of magnetization

High spin molecules as quantum processors

Quantum computing in molecular magnets

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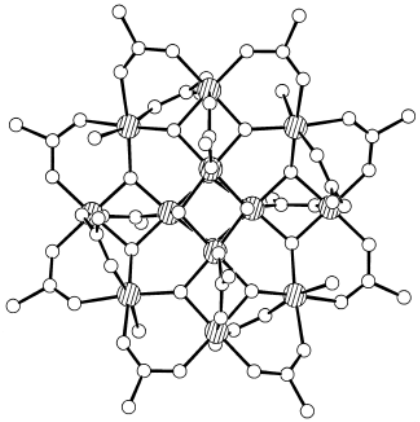
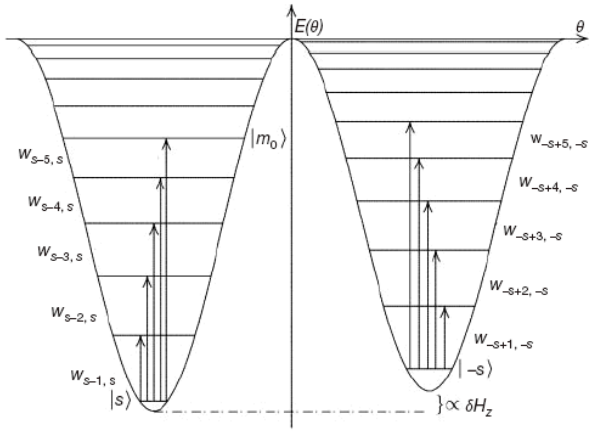
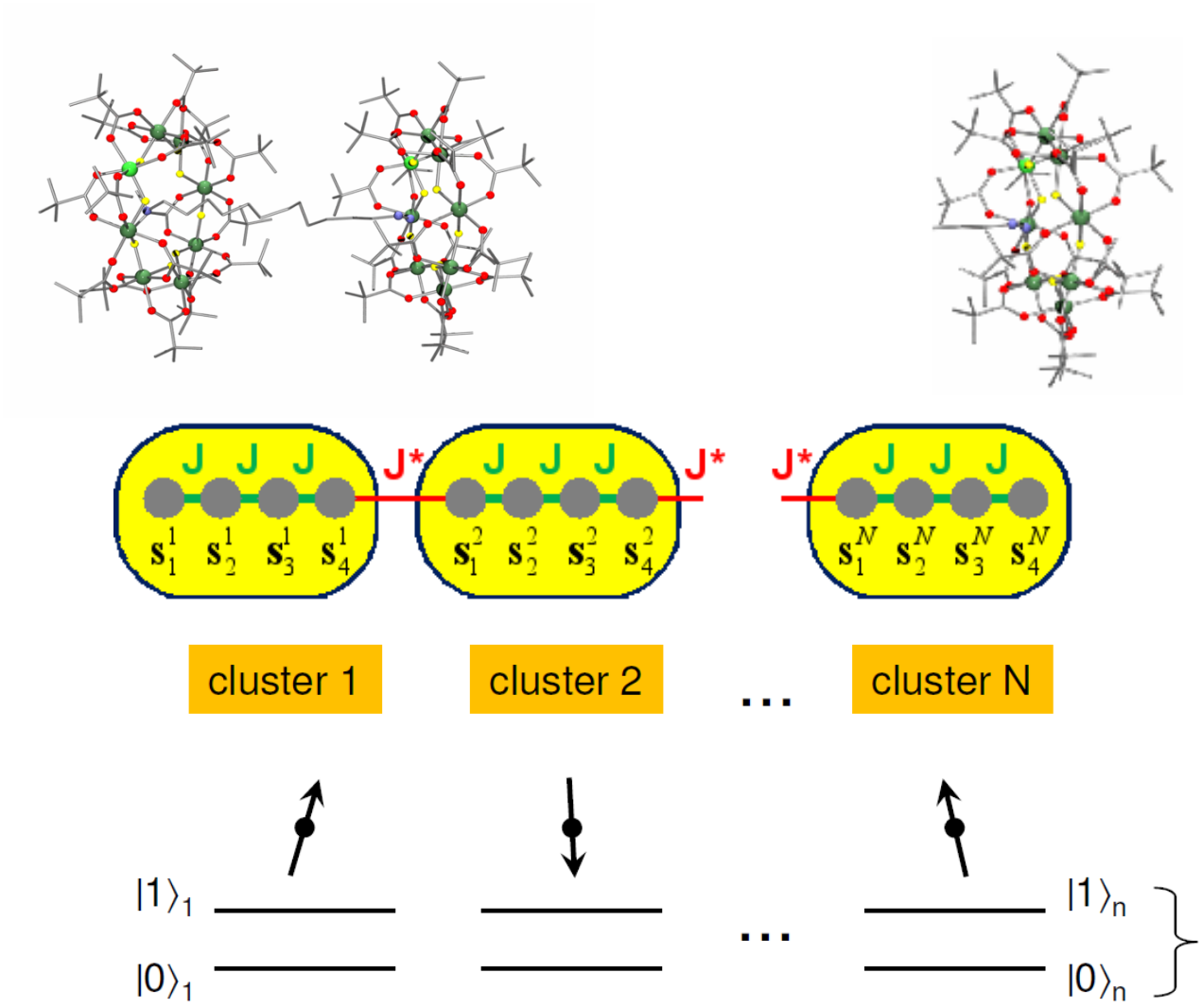
Shor and Grover demonstrated that a quantum computer can outperform any classical computer in factoring numbers[1] and in searching a database[2] by exploiting the parallelism of quantum mechanics. Whereas Shor's algorithm requires both superposition and entanglement of a many-particle system[3], the superposition of single-particle quantum states is sufficient for Grover's algorithm[4]. Recently, the latter has been successfully implemented[5] using Rydberg atoms. Here we propose an implementation of Grover's algorithm that uses molecular magnets[6–10], which are solid-state systems with a large spin; their spin eigenstates make them natural candidates for single-particle systems. We show theoretically that molecular magnets can be used to build dense and efficient memory devices based on the Grover algorithm. In particular, one single crystal can serve as a storage unit of a dynamic random access memory device. Fast electron spin resonance pulses can be used to decode and read out stored numbers of up to 10^5, with access times as short as 10^{-10} seconds. We show that our proposal should be feasible using the molecular magnets Fe_8 and Mn_{12}.



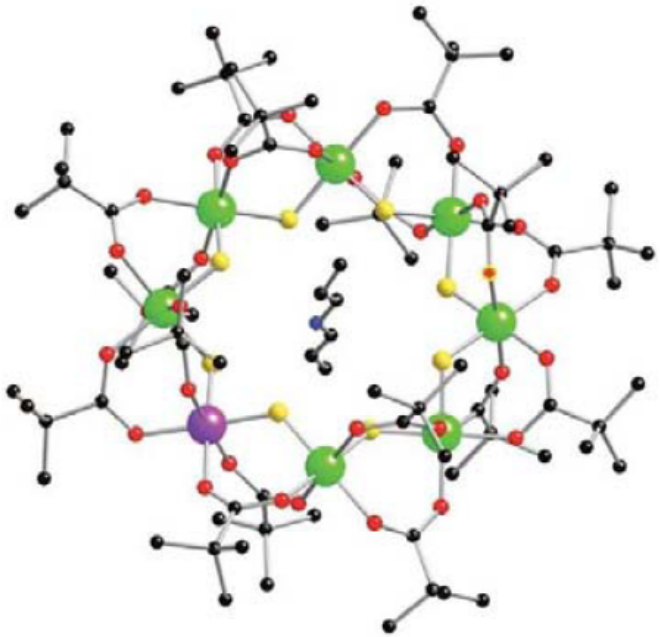


Low spin molecules as spin cluster qubits



Meier, Levy, Loss, Phys. Rev. Lett. 90, 047901 (2003)

Single molecule Cr_7Ni



Crystallographic structure of Cr7Ni "green" obtained from X-ray diffraction

diameter $\sim$ 1 nm
7 Cr (green), 1 Ni (purple), 8 F (yellow),
32 O (red), 80 C (black), 144 H (-)

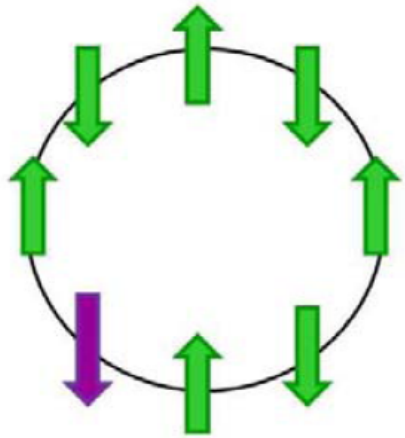
Well studied system

NMR: Micotti, et al., PRL 97, 267204 (2006)
EPR: Ardavaran et al., PRL 98, 57201 (2007)
XMCD: Corradini et al., PRB 77, 014402 (2008)

$\vdots$

Robust magnetic core

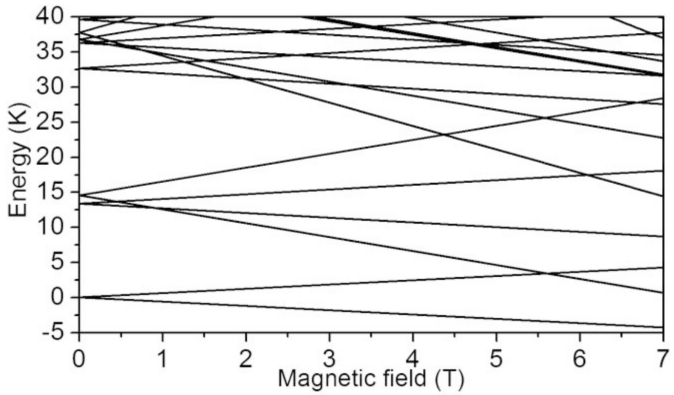
$$S_{Cr} = 3/2, \qquad S_{Ni} = 1$$



Sketch of the spin arrangement in the molecule
(from the Phd thesis of G. Lorusso)

The electron spin degrees of freedom

$$H_e = \sum_{i=1}^{8} J_i \mathbf{s}_i \cdot \mathbf{s}_{i+1} + \sum_{i=1}^{8} d_i [s_{z,i}^2 - s_i(s_i+1)/3] + \sum_{i<j=1}^{8} \mathbf{s}_i \cdot \mathbf{D}_{ij} \cdot \mathbf{s}_j + \mu_B \sum_{i=1}^{8} g_i \mathbf{B} \cdot \mathbf{s}_i \qquad (1)$$



- Well separated degenerate ground state. $\Delta(0) \simeq 13K$.
- Well resolved ground state.
- Optimal operating point at around 2 T. $\Delta(B_0) \simeq \Delta(0) - 2g\mu_B B_0 \simeq 9.4K$.

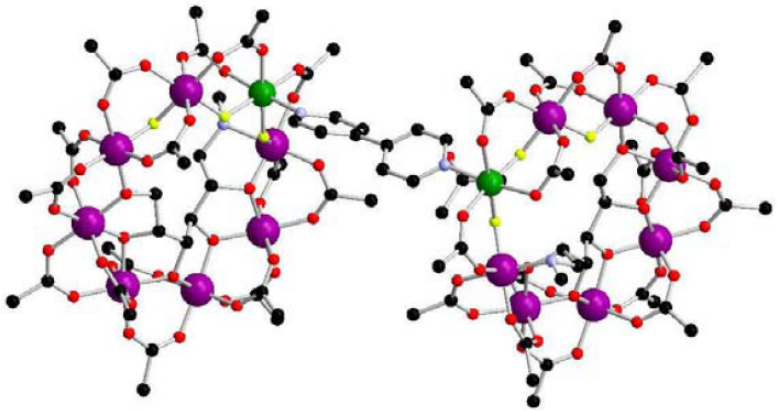
The ground state degeneracy behaves like a **S=1/2 spin** system.

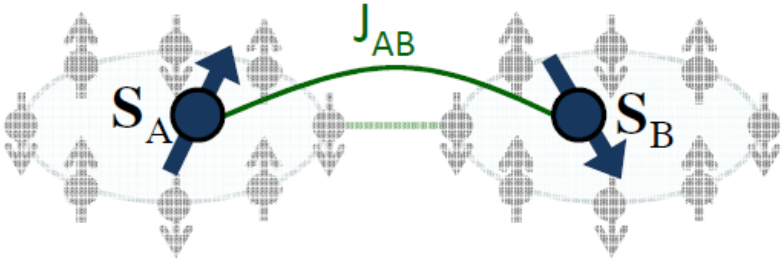
$$|\Uparrow> \equiv |S = 1/2, M = 1/2>$$

$$|\Downarrow> \equiv |S = 1/2, M = -1/2>$$

F. Troiani, A. Ghirri, M. Affronte et al., Phys. Rev. Lett. 94, 207208 (2005)

The model





Projected electron spin Hamiltonian

$$H_Z^{\chi=A,B} = \mu_B g_\chi \mathbf{S}_z^\chi$$

$$H_{ex}^{AB} = J_{AB} \mathbf{S}_A \mathbf{S}_B$$

$$J_{AB} \approx 0.16K$$

$$J_k \approx 23K$$

$\Longrightarrow$ for the single molecule Hamiltonian the inter ring coupling is **perturbative**

hyperfine

$$H_{en} = \sum_l \sum_k E_{kl}^{\alpha\beta} S_k^\alpha I_k^\beta$$

nuclear spins

$$H_n = -\sum_k B\gamma_k I_k + \sum_{k<l} D_{kl}^{\alpha\beta} I_k^\alpha I_l^\beta$$

Timco, et al. Angewandte Chemie **47** 9681

Effective Hamiltonian

$$H_Z^{\chi=A,B} \gg |H_{en}|$$

Applying high external magnetic field $\Longrightarrow$ Energy relaxation is strongly inhibited

$\Longrightarrow |S, M\rangle$ (with $\mathbf{S} = \mathbf{S}_A + \mathbf{S}_B$) is a **good quantum number**

Effective Hamiltonian

- obtained by a standard canonical transformation
- the second-order correction of the off diagonal terms is reduced
- keep only momentum conserving terms of the Hamiltonian

$$\mathcal{H}_{\text{eff}} = \sigma_z^e \otimes \mathcal{H}_n^{(e)} + \mathcal{I}^e \otimes \mathcal{H}_n^{(i)}, \tag{2}$$

where

$$\sigma_z^e \equiv |S_1, M_1\rangle\langle S_1, M_1| - |S_2, M_2\rangle\langle S_2, M_2| \qquad \mathcal{I}^e \equiv |S_1, M_1\rangle\langle S_1, M_1| + |S_2, M_2\rangle\langle S_2, M_2|$$

$$\mathcal{H}_n^{(\alpha)} = \sum_{k=1}^{N_n} A_k^{(\alpha)} I_k^z + \sum_{k,l=1}^{N_n} \left[B_{kl}^{(\alpha)} I_k^z I_l^z + C_{kl}^{(\alpha)} I_k^+ I_l^- \right], \tag{3}$$

Pure dephasing of the electron state

Hamiltonians:

$$H = H_S + H_{SE} + H_E$$

$$H_S = E_1^0 |\psi_1\rangle\langle\psi_1| + E_2^0 |\psi_2\rangle\langle\psi_2|$$

$$H_{SE} = |\psi_1\rangle\langle\psi_1| \otimes H_{SE}^1 + |\psi_2\rangle\langle\psi_2| \otimes H_{SE}^2$$

$$H_{SE} \neq 0, \qquad [H_S, H_{SE}] \approx 0, \qquad [H_E, H_{SE}] \neq 0$$

Time evolution:

$$|\Psi_0\rangle = |\Psi_{e0}\rangle \otimes |\Psi_{n0}\rangle \longrightarrow |\Psi_t\rangle$$

$$\frac{1}{\sqrt{2}} \left(|S_1, M_1\rangle + |S_2, M_2\rangle\right) \otimes |\mathbf{I}\rangle \longrightarrow \frac{1}{\sqrt{2}} \left[|S_1, M_1\rangle \otimes |\mathbf{I}_1(t)\rangle + e^{i\phi_{\mathbf{I}}(t)} |S_2, M_2\rangle \otimes |\mathbf{I}_2(t)\rangle\right]$$

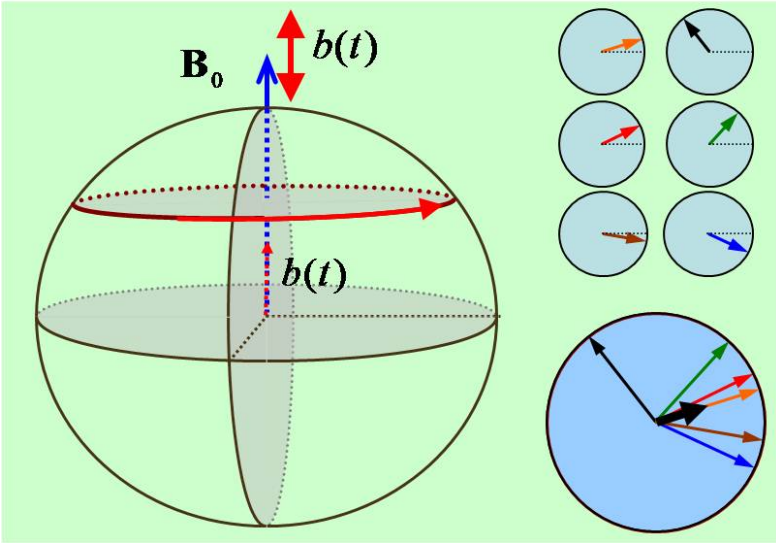
The electron-spin decoherence is induced by the correlation between the electron-state and nuclear bath.

$$\begin{aligned} \rho_e(t) &= \mathrm{Tr}_n \left\{|\Psi_t\rangle\langle\Psi_t|\right\} = \frac{1}{2} \sum_{k=1,2} |S_k, M_k\rangle\langle S_k, M_k| \\ &+ \frac{r_{\mathbf{I}}(t)}{2} \left[|S_2, M_2\rangle\langle S_1, M_1| e^{i\phi_{\mathbf{I}}(t)} + \mathrm{h.c.}\right], \qquad (4) \\ & r_{\mathbf{I}} = |\langle \mathbf{I}_1 | \mathbf{I}_2 \rangle|, \; \phi_{\mathbf{I}} = \arg\{\langle \mathbf{I}_1 | \mathbf{I}_2 \rangle\} \end{aligned}$$

Inhomogeneous broadening

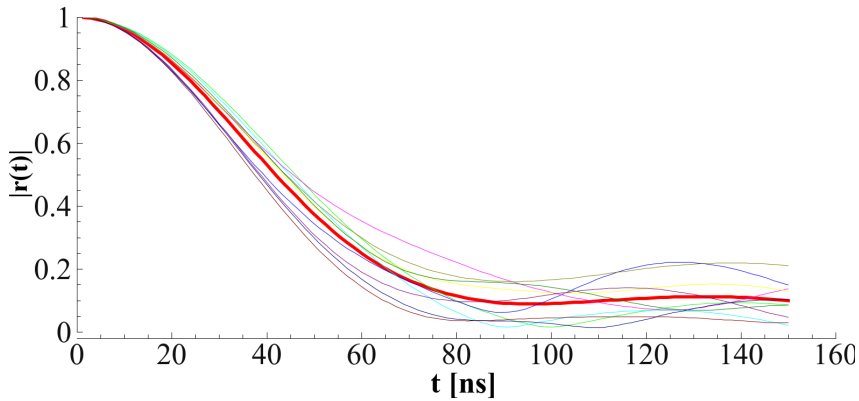
Initial electron state: $|\Psi_0\rangle = \frac{1}{\sqrt{2}}(|T_+\rangle + |T_-\rangle)$ (Bell state)

Semiclassical picture:

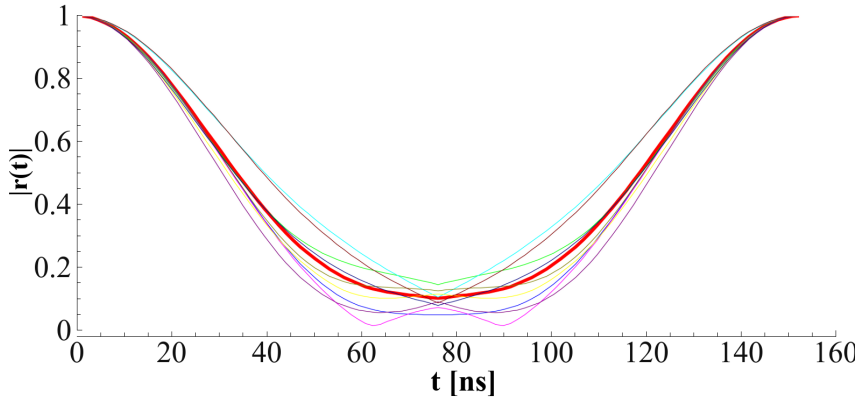


from R. B. Liu, Department of Physics,
The Chinese University of Hong Kong

Free induction decay



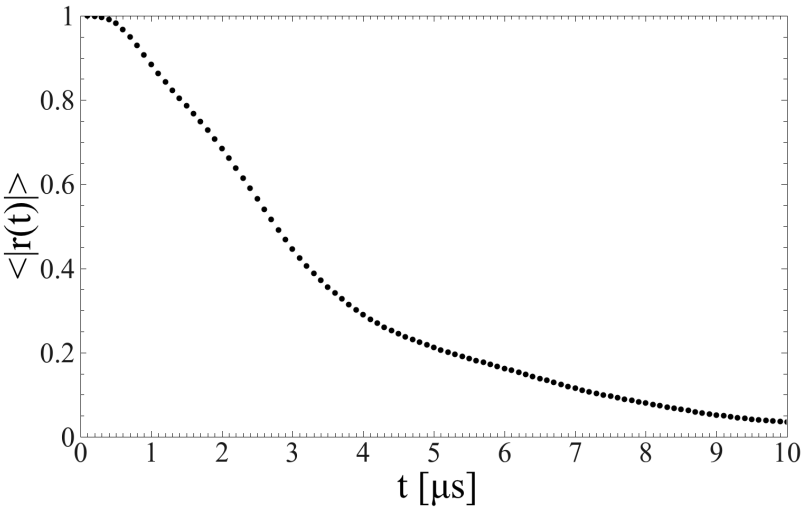
The effect of a π pulse: Hahn echo

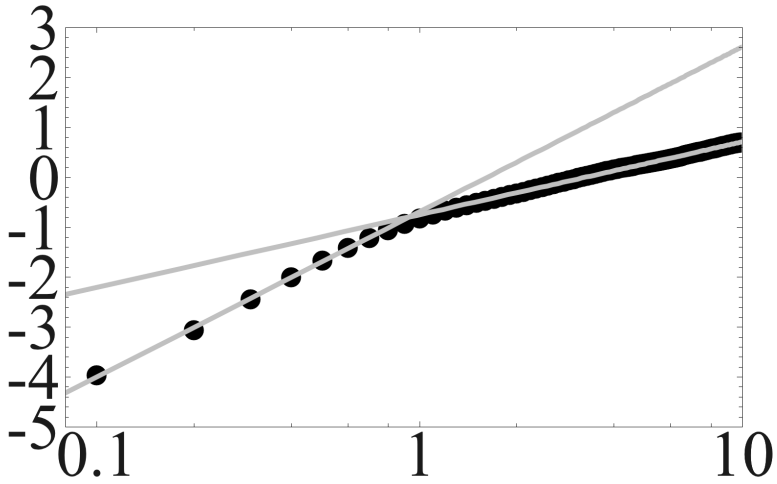


- Decoherence on the nanosecond timescale
- Possible to fully recover with Hahn echo

Coherence decay rate

Initial electron state: $|\Psi_0\rangle = \frac{1}{\sqrt{2}}(|T_+\rangle + |T_-\rangle)$





Exponential decay $r(t) = \exp\{-(t/\tau_d)^\alpha\}$

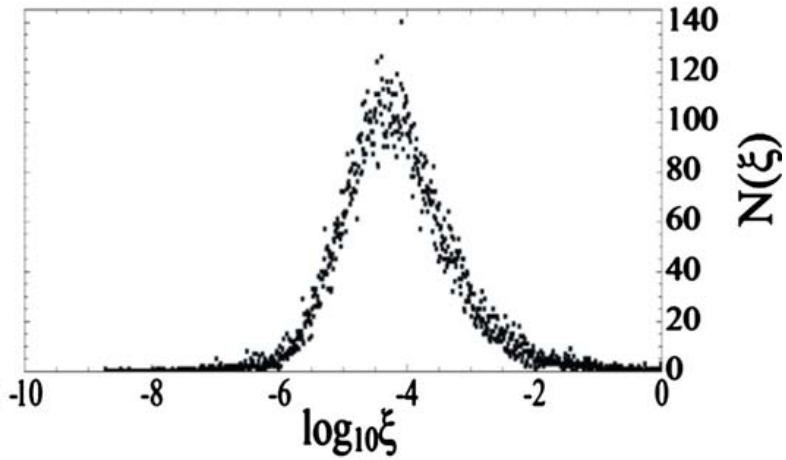
Two distinct regimes can be clearly identified:

I. $t \lesssim 1\,\mu$s, $\alpha = 3.31$ and $\tau_d = 1.65\,\mu$s

II. $t \gtrsim 1\,\mu$s, $\alpha = 1.46$ and $\tau_d = 3.24\,\mu$s

The origin of the two regimes is the existence of the different types of nuclear pairs

I. very few closely located pairs
II. huge number of pairs located far from each other



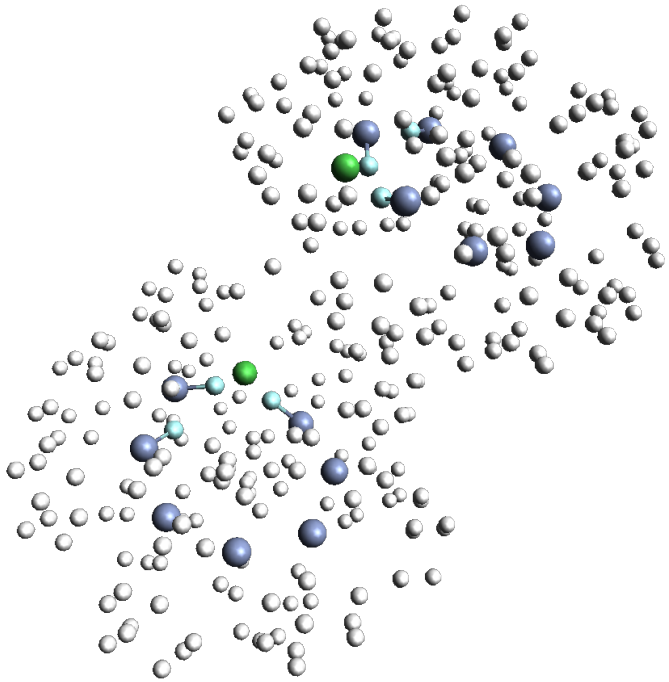
$$\xi \equiv |C_{kl}^{(i)}| / [(C_{kl}^{(i)})^2 + (A_k^{(e)} - A_l^{(e)})^2]^{1/2}$$

Chemical elements dependence of the decoherence

Initial electron state: $|\Psi_0\rangle = \frac{1}{\sqrt{2}}(|T_+\rangle + |T_-\rangle)$

Which chemical elements dominate the decoherence?

- the few fluorines that located close to the electron spin
- the numerous hydrogens that located far away ($> 4\mathring{A}$) from the electron spins



The decoherence is dominated by the **hydrogens**.
However practically all the decoherence is originated from the intra molecular couplings and not from the inter molecular ones.

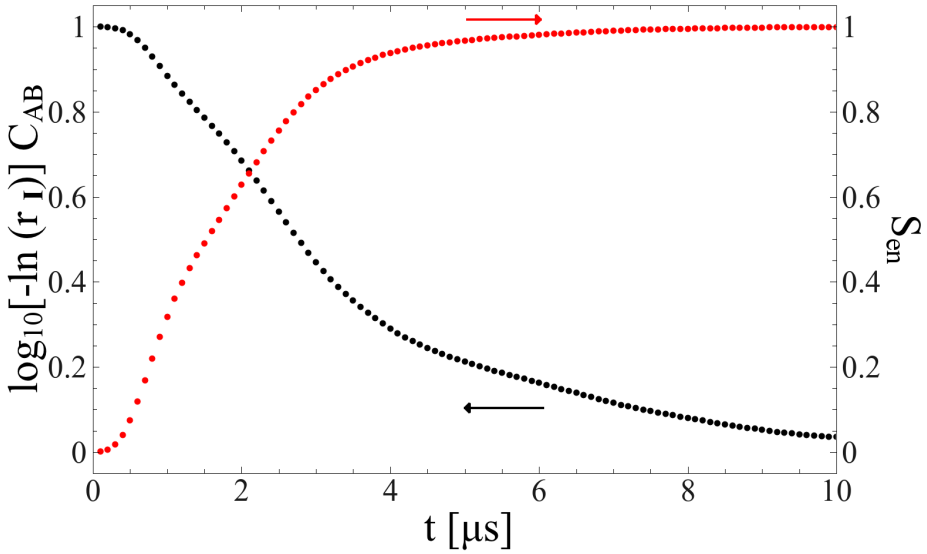
Entanglement properties

concurrence
between the two qubits (for the density matrix ρ_e):

$$\mathcal{C}_{AB}(\rho_e) = r_{\mathbf{I}}. \tag{5}$$

the von Neumann entropy
between electron and nuclear spins:

$$S_{en}(\rho_e) = -\frac{1}{2}\sum_{\mu=\pm 1}(1+\mu r_{\mathbf{I}})\log_2\left[\frac{1}{2}(1+\mu r_{\mathbf{I}})\right]. \tag{6}$$

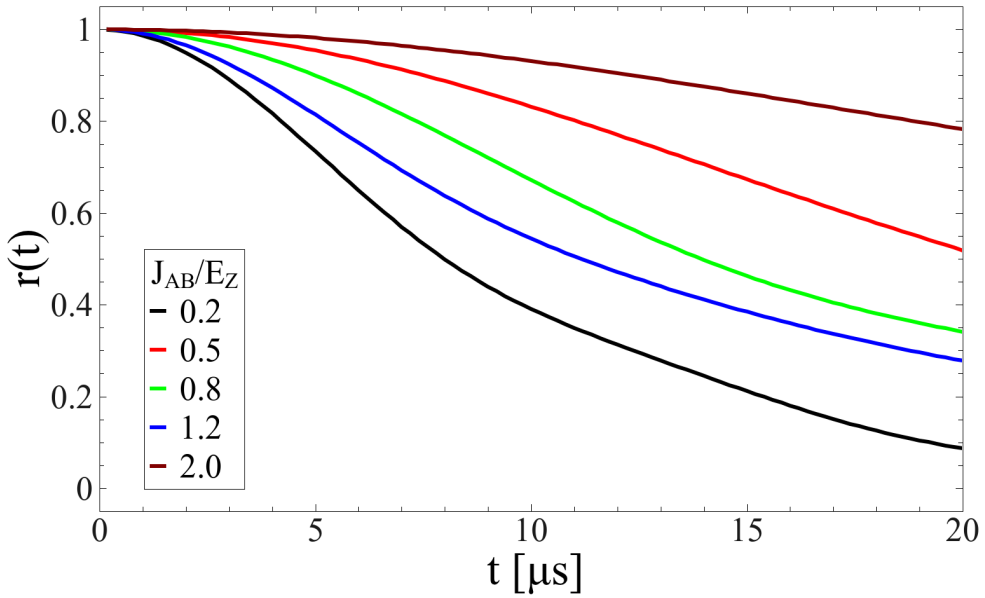


Mutually exclusive nature of electron-nuclear and intermolecular entanglement

Singlet Triplet decoherence

Different linear combination of the electron states:

$$|\Psi_0\rangle = \frac{1}{\sqrt{2}}(|S\rangle + |T_0\rangle)$$



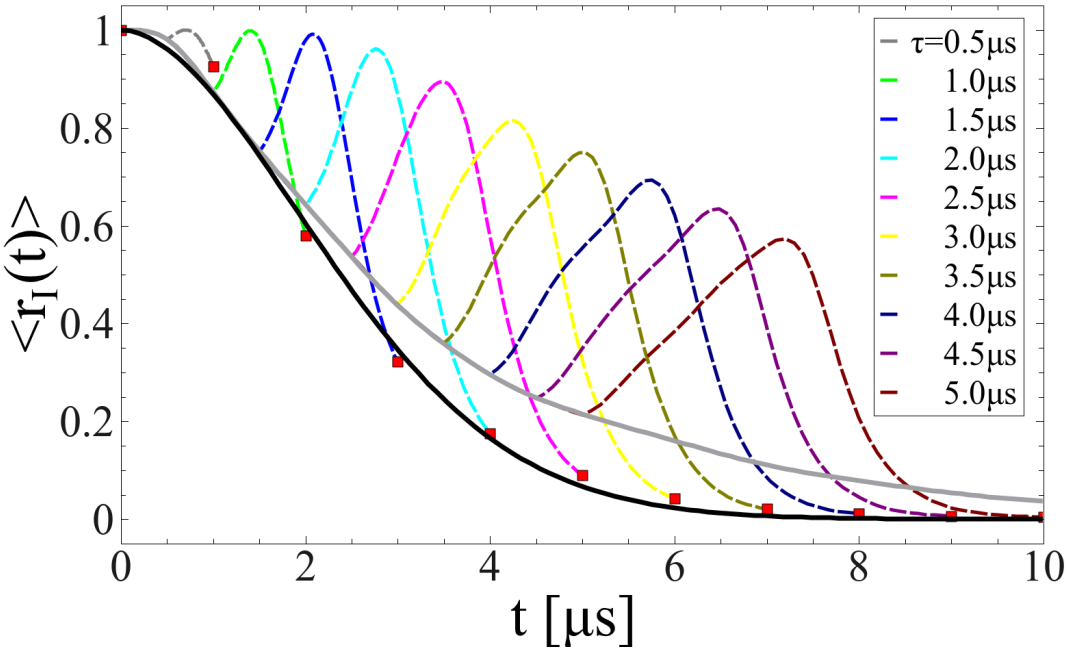
- Fundamentally different features compared to the Bell state ⇒ much slower decoherence rate compare to the Bell state
- The time-evolution of r is strongly dependent on the intermolecular exchange J_{AB}
- The decoherence is caused by the **fluorines**
- The decoherence rate decreases for increasing energy difference between the singlet state and each of the triplet states
- Decoherence free subspace for the system

The density matrix in this case is always factorizable into the states of $\mathbf{S}_A$ and $\mathbf{S}_B$: $\mathcal{C}_{AB}(\rho_e) = 0$.

A. Szallas and F. Troiani, Phys. Rev. B **82** 224409 (2010)

Dynamical decoupling

Partial recovery of the electron spin coherence



The effect on decoherence by entanglement of a flip of the electron spins $\mathbf{S}_{\chi=A,B}$ at a time $t = \tau$ that can be induced by an EPR π-pulse.

- Maximum recovery at $t \simeq \sqrt{2}\tau$
- Stronger electron - nuclear correlation at $t = 2\tau$ (red squares) than those obtained in the absence of the $\pi-$pulse (brown curve)

Conclusions

- Bell state decoherence is driven by the interplay between intrinsic nuclear interactions (H nuclei) and electron-spin induced magnetic field
- singlet-triplet decoherence has longer timescales, and is driven by second-order processes involving F nuclei
- electron and nuclear spins can be partially disentangled by spin-echo sequences

Köszönöm a figyelmet!