

Toroidal magnetic molecules stripped to their basics

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Imagine ...

Imagine someone tells you that
toroidal magnetic molecules
are superb building blocks
of quantum devices.

JS

What are toroidal magnetic molecules good for?



Toroidal magnetic molecules are molecules that possess a magnetic moment that is shaped like a torus. These molecules have unique magnetic properties that make them potentially useful for a variety of applications, particularly in the fields of nanotechnology and spintronics.

One potential application of toroidal magnetic molecules is in the development of magnetic data storage devices. The toroidal magnetic moment of these molecules can be used to store data in a highly compact and efficient manner, making them ideal for use in future generations of hard drives or other magnetic memory devices.

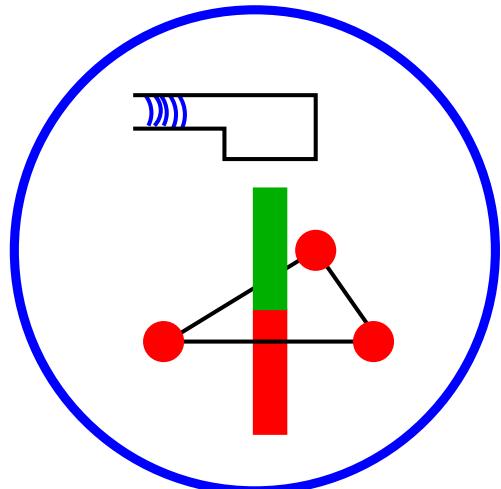
Another potential application of toroidal magnetic molecules is in the field of quantum computing. The unique magnetic properties of these molecules could potentially be used to develop new types of qubits, which are the building blocks of quantum computers. Toroidal magnetic molecules could also be used to create topologically protected qubits, which are more robust against external disturbances than traditional qubits.

Would you buy one?

Or would you first check
such molecules?

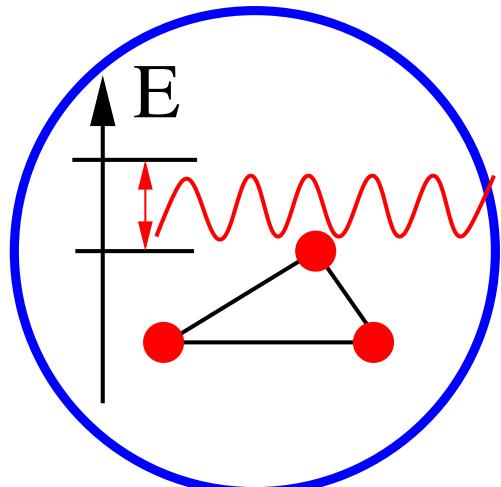
And if, what would you
investigate?

Quantum devices – figures of merit



Memory unit

- requires bistability
- problem 1: quantum tunneling
- problem 2: stability against field fluctuations



Q-bit

- requires coherence
- problem decoherence

Yes, we can!

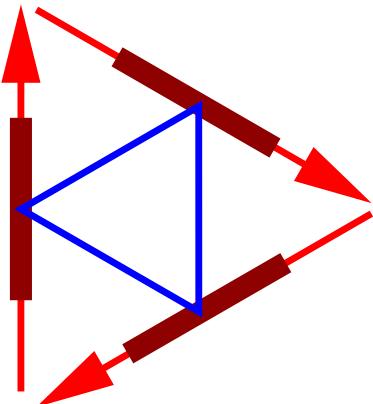

$$\begin{pmatrix} 3 & 42 & 4711 \\ 42 & 0 & 3.14 \\ 4711 & 3.14 & 8 \\ -17 & 007 & 13 \\ 1.8 & 15 & 081 \end{pmatrix}$$

1. Toroidal magnetic molecules
2. Bistability, tunneling, and stability
3. Clock transitions and decoherence

We are the sledgehammer team of matrix diagonalization.
Please send inquiries to jschnack@uni-bielefeld.de!

Toroidal magnetic molecules

Torodial magnetic molecules I

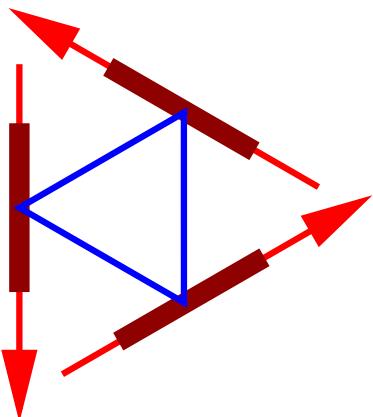


Toroidal magnetic moment

$$\vec{\tau} = \sum_i \vec{r}_i \times \vec{s}_i$$

Model Hamiltonian I

$$\begin{aligned} H = & -2 \sum_{i < j} J_{ij} \vec{s}_i \cdot \vec{s}_j + D \sum_i \left(\vec{s}_i \cdot \vec{e}_i^3 \right)^2 \\ & + \mu_B g \vec{B} \cdot \sum_i \vec{s}_i \end{aligned}$$



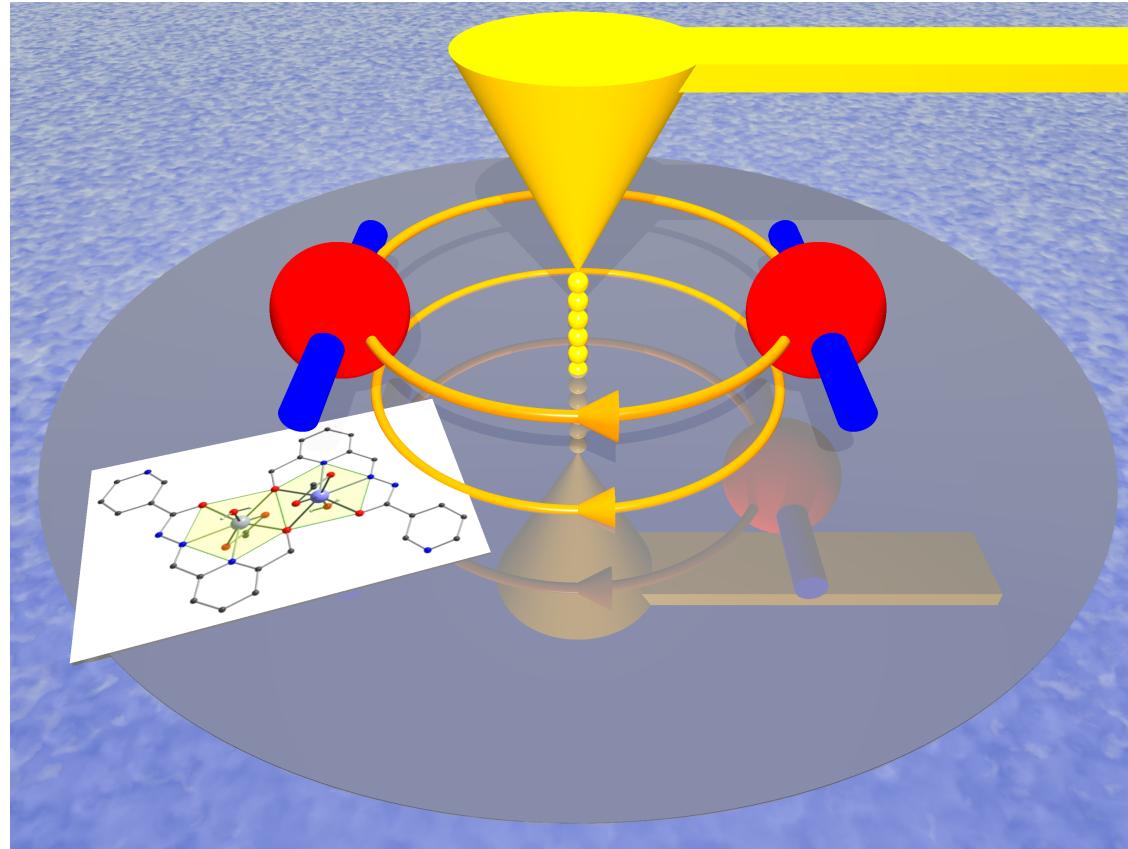
Classical ground states with vanishing moment, but non-vanishing toroidal moment.

J. Tang, I. Hewitt, N. T. Madhu, G. Chastanet, W. Wernsdorfer, C. E. Anson, C. Benelli, R. Sessoli, and A. K. Powell, *Angew. Chem. Int. Ed.* **45**, 1729 (2006).

A. Soncini and L. F. Chibotaru, *Phys. Rev. B* **77**, 220406 (2008).

D. Pister, K. Irländer, D. Westerbeck, and J. Schnack, *Phys. Rev. Research* **4**, 033221 (2022).

Torodial magnetic molecules II

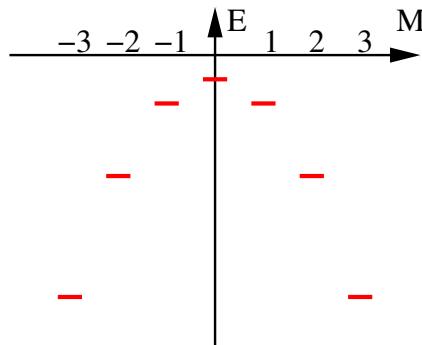


D. Pister, K. Irländer, D. Westerbeck, and J. Schnack, Phys. Rev. Research **4**, 033221 (2022).

Bistability, tunneling, and stability

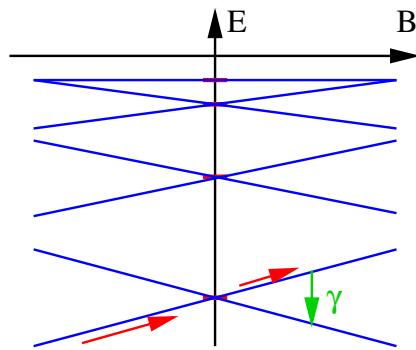
(Remember what we know from SMMs!)

Single-ion anisotropy and bistability I – good SMM



$$\tilde{H} = \sum_i D_i (\xi_i^z)^2 + \mu_B B \sum_i g_i \xi_i^z + \tilde{H}_{\text{ferro int}}$$

$D_i < 0$ collinear easy axes

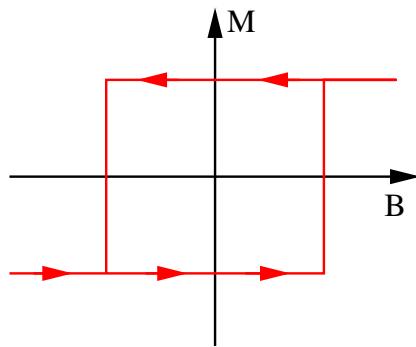


eigenvectors: $|S, M, \alpha\rangle$

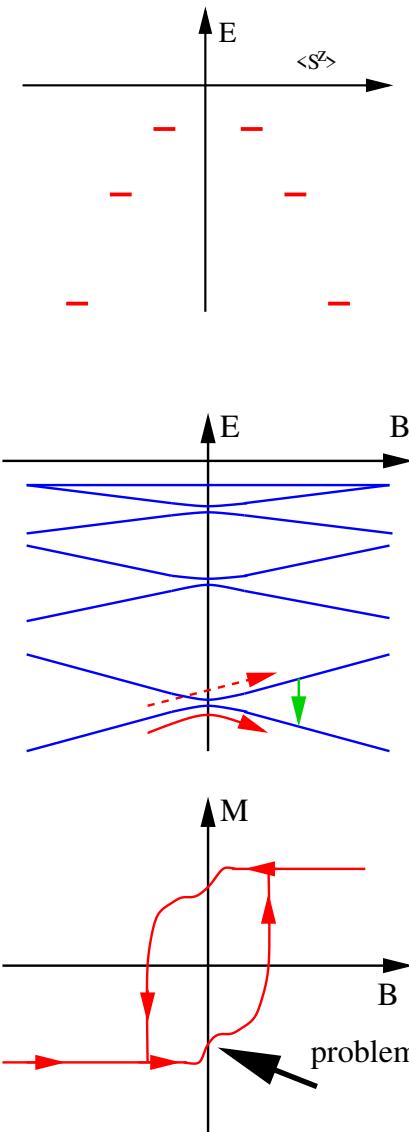
low-lying eigenvalues: $E_M = DM^2 + g\mu_B BM$

IMPORTANT: $[\tilde{H}, \xi^z] = 0$ since all D tensors aligned!!!

⇒ level crossings at $B = 0$
 ⇒ good hysteresis



Single-ion anisotropy and bistability II – bad/no SMM



$$\tilde{H} = \sum_i \vec{s}_i \cdot \mathbf{D}_i \cdot \vec{s}_i + \mu_B B \sum_i g_i s_i^z + H_{\text{ferro int}}$$

\mathbf{D}_i individual non-collinear anisotropy tensors

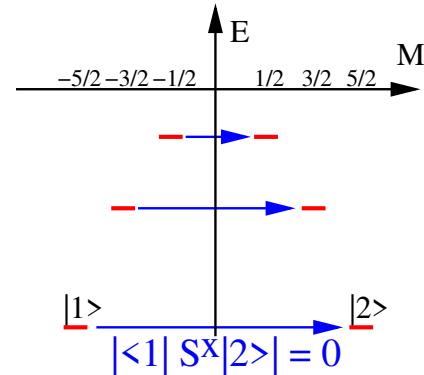
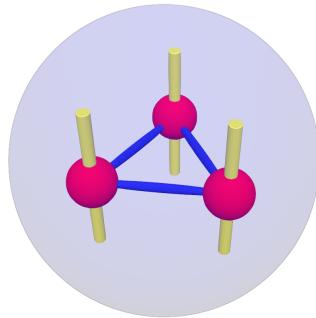
NO LONGER eigenvectors: $|S, M, \alpha\rangle$

low-lying eigenvalues only approx. parabola (if at all)

IMPORTANT: $[\tilde{H}, \tilde{s}^z] \neq 0$

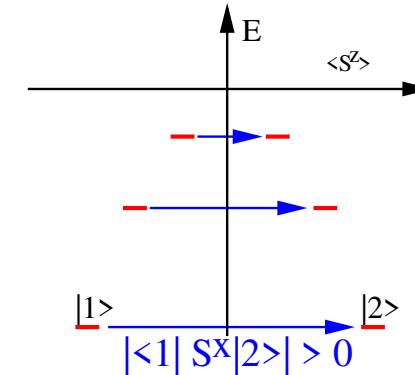
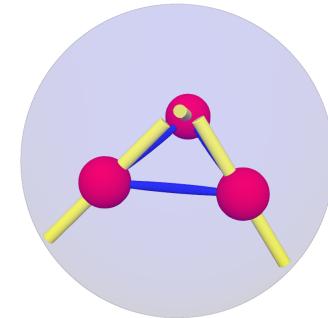
⇒ avoided level crossings at $B = 0$ for integer spins
 ⇒ poor/no hysteresis – not bistable & bad for storage

Single-ion anisotropy and bistability III – stability



Collinear easy axes:

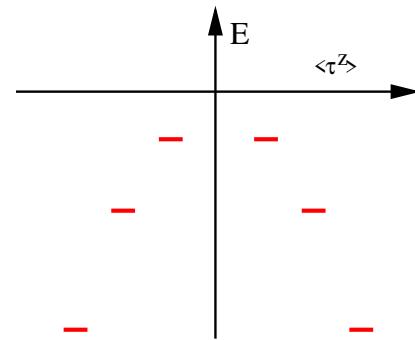
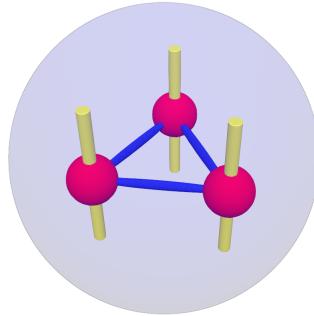
- ⇒ No tunneling gap
- ⇒ No transition matrix elements



Non-collinear easy axes:

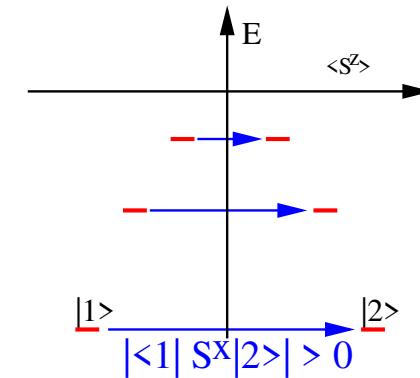
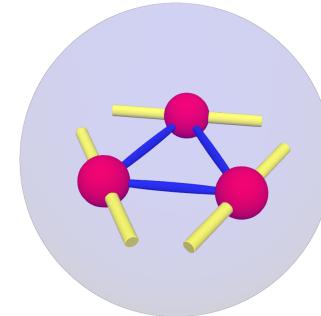
- ⇒ Tunneling gap for integer spin
- ⇒ (large) Transition matrix elements

Single-ion anisotropy and bistability IV – stability



Collinear easy axes:

- ⇒ No tunneling gap
- ⇒ No transition matrix elements



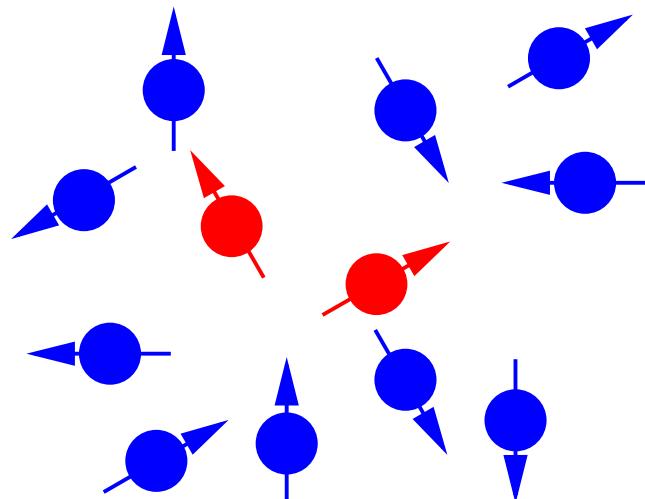
Non-collinear easy axes:

- ⇒ Tunneling gap for integer spin
- ⇒ (large) Transition matrix elements

Toroidal moments are here!

Stability of (toroidal) clock transitions

Context



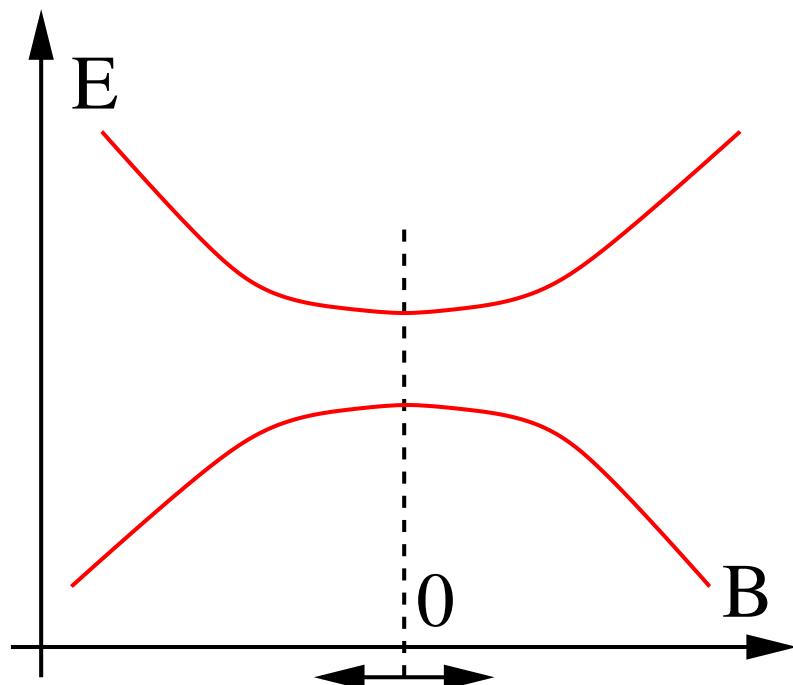
Investigation of **decoherence of a subsystem** if the combined system (including bath) is evolved via the time-dependent Schrödinger equation.

Employed measure of decoherence: reduced density matrix

$$\tilde{\rho}_{\text{system}} = \text{Tr}_{\text{bath}} (\tilde{\rho})$$

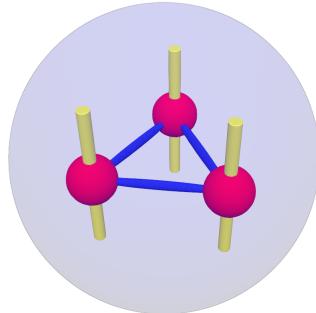
Typically: unitary-time evolution of pure state approximates dynamics of density matrix.

Concept of clock transitions



Fluctuations of B produce little effect on dynamics of superposition since ΔE of clock transition is independent of field at $B = 0$, at least to some order of a Taylor expansion.

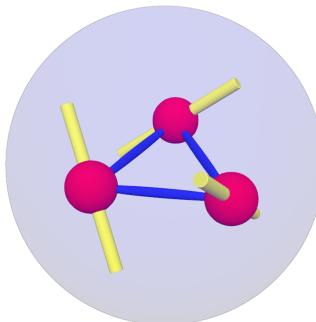
Clock transitions with toroidal magnetic molecules



Model Hamiltonian II

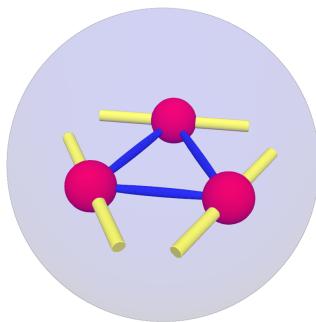
$$\begin{aligned}\tilde{H} = & -2 \sum_{i < j} J_{ij} \tilde{s}_i \cdot \tilde{s}_j + D \sum_i \left(\tilde{s}_i \cdot \vec{e}_i^3 \right)^2 \\ & + \mu_B g \vec{B} \cdot \sum_i \tilde{s}_i + \tilde{H}_{\text{int}} + \tilde{H}_{\text{bath}}\end{aligned}$$

Reasonable parameters: weak J , strong D .
Dipolar interactions with and among 8 ... 10 bath spins.



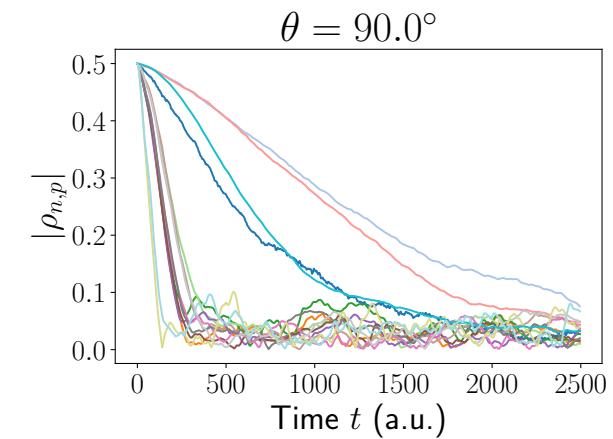
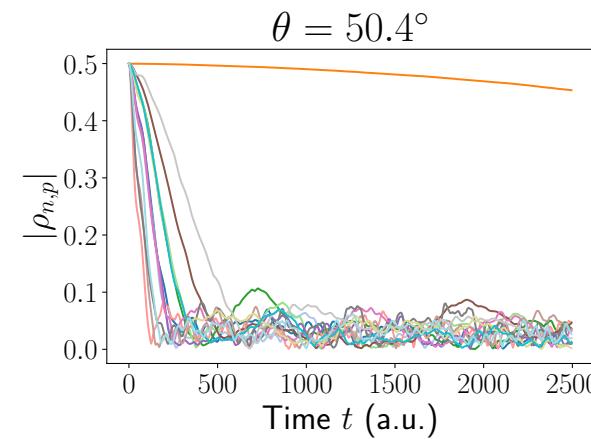
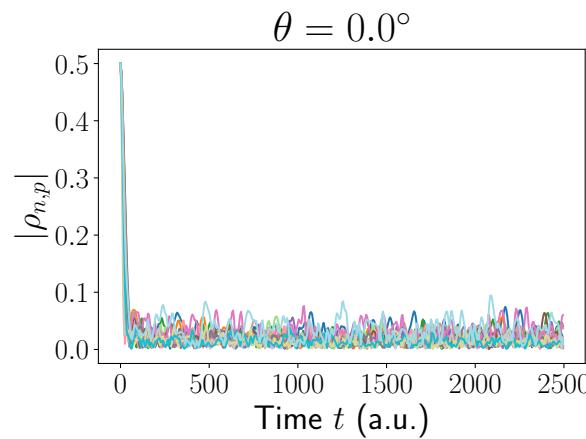
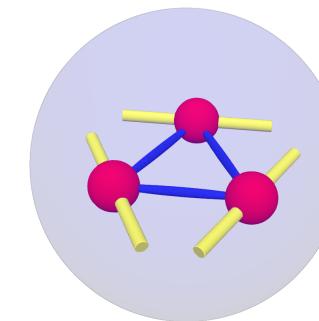
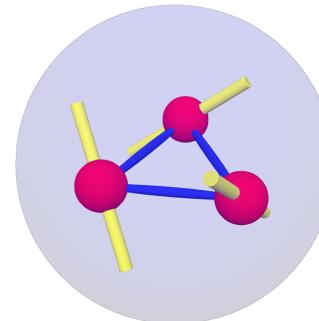
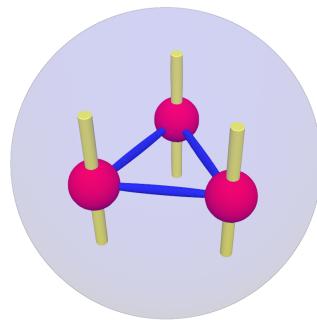
Investigation as function of tilt angle

- various clock transitions of the spectrum,
- various arrangements of the decohering bath.



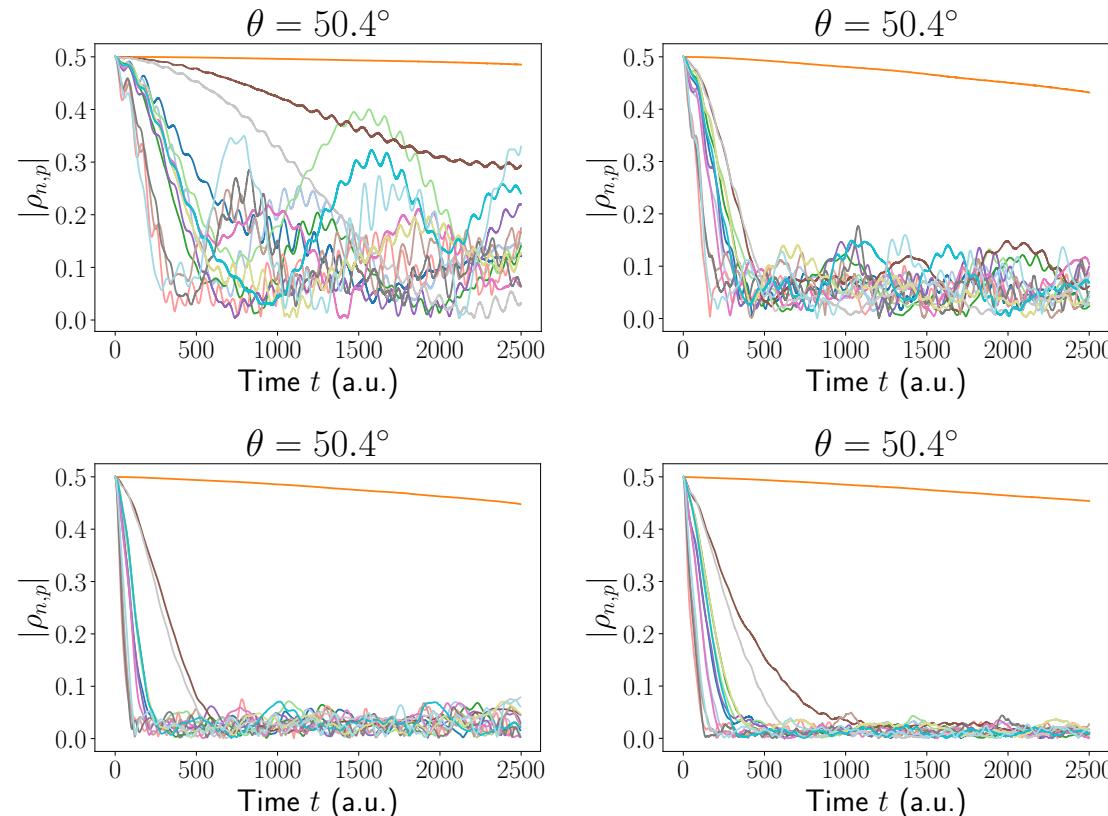
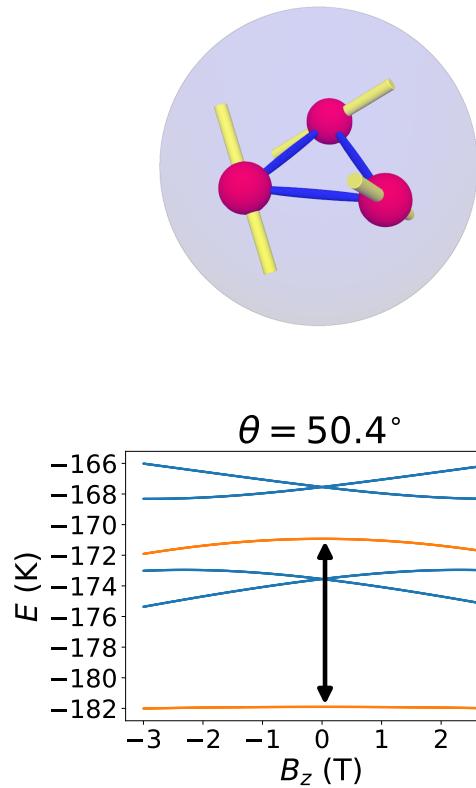
K. Irländer, J. Schnack, Phys. Rev. Research **5**, 013192 (2023).

Clock transitions with toroidal magnetic molecules



K. Irländer, J. Schnack, Phys. Rev. Research 5, 013192 (2023).

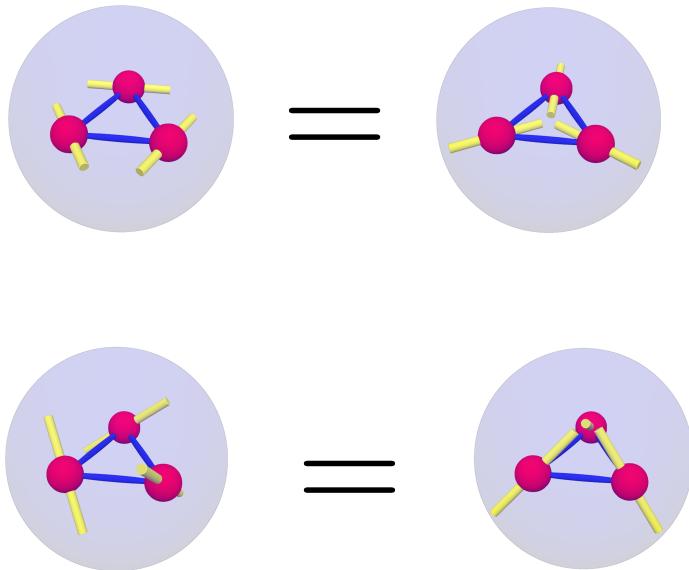
Clock transitions with toroidal magnetic molecules



Decoherence as function of size of the bath (4, 6, 8, 10).

K. Irländer, J. Schnack, Phys. Rev. Research 5, 013192 (2023).

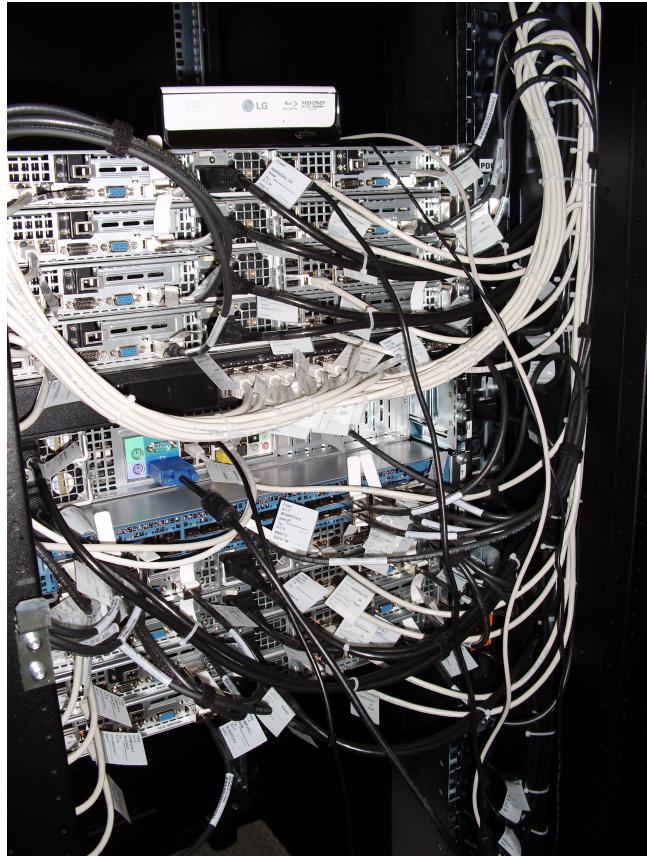
Decoherence of toroidal magnetic molecules



- Toroidal structure irrelevant, i.e. not correlated with desired properties.
- Canted, near orthogonal anisotropy axes optimal in our example.
- Dipolar interactions between system spins do not alter the picture.

K. Irländer, J. Schnack, Phys. Rev. Research **5**, 013192 (2023).

Summary



- Toroidal magnetic molecules: perspectives not clear (to me).
- Relaxation measurements needed!
- Decoherence measurements needed!
- More theory needed to e.g. assess the influence of anisotropic interactions.

Many thanks to my collaborators



- C. Beckmann, M. Czopnik, T. Glaser, O. Hanebaum, Chr. Heesing, M. Höck, K. Irländer, N.B. Ivanov, H.-T. Langwald, A. Müller, H. Schlüter, R. Schnalle, Chr. Schröder, J. Ummethum, P. Vorndamme, D. Westerbeck (Bielefeld)
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Thank you very much for your
attention.

The end.

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