Spinsysteme, magnetische Moleküle, Quantencomputer und noch mehr Magnetismus – Teil I

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Yes, we can!

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

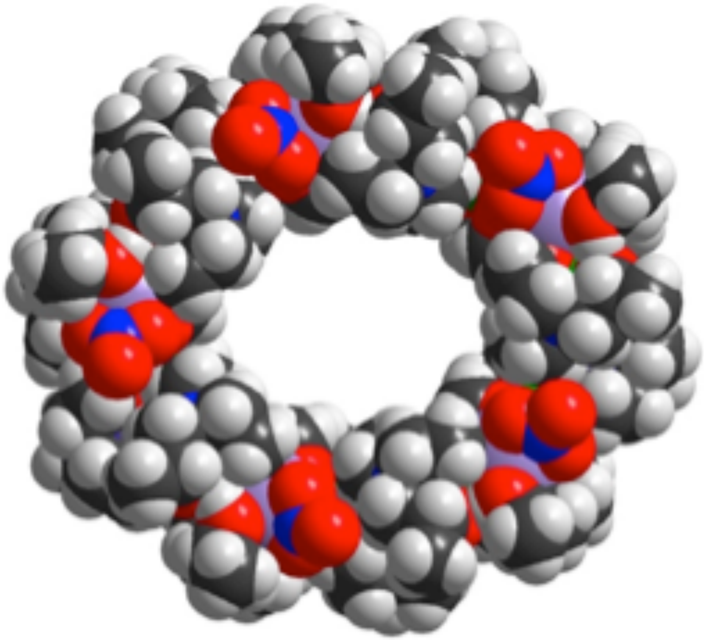
1. A flash on magnetic molecules
2. Typicality approach to equilibrium
3. Studies on decoherence
4. Spin-phonon issues
5. Bachelor and Master theses

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

We investigate magnetic molecules

J. Schnack, Contemporary Physics **60**, 127-144 (2019)

You have got a molecule!

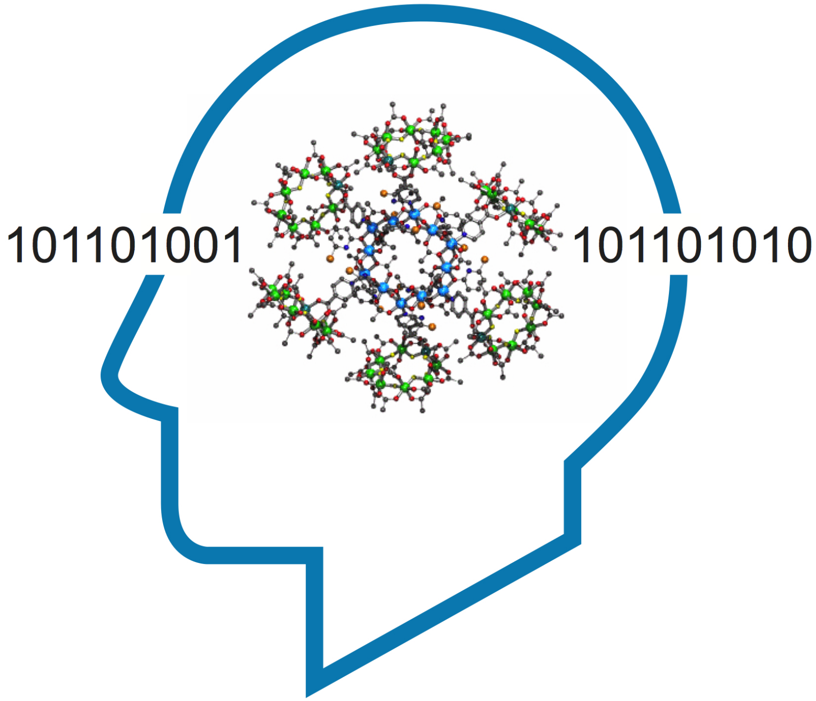


$S = 60$

Congratulations!

Powell group: npj Quantum Materials **3**, 10 (2018)

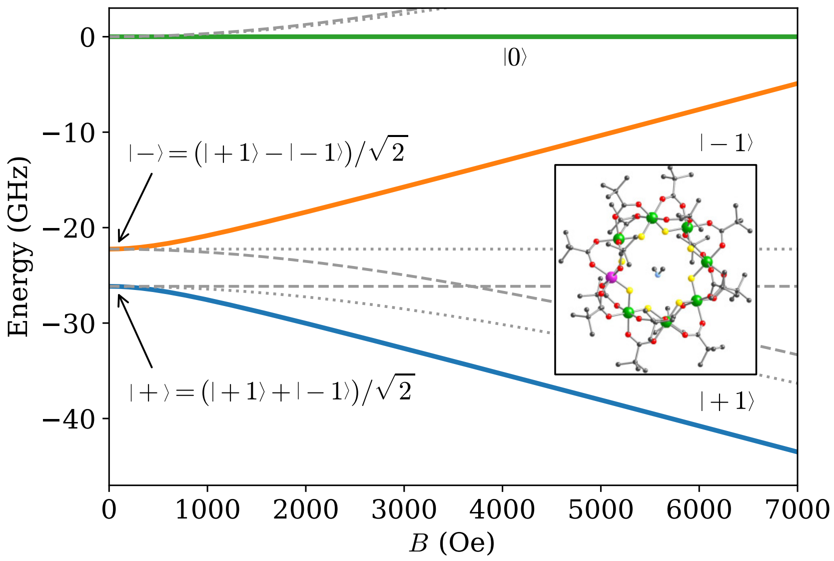
You want to build a quantum computer!



Very smart!

Wernsdorfer group: Phys. Rev. Lett. **119**, 187702 (2017)

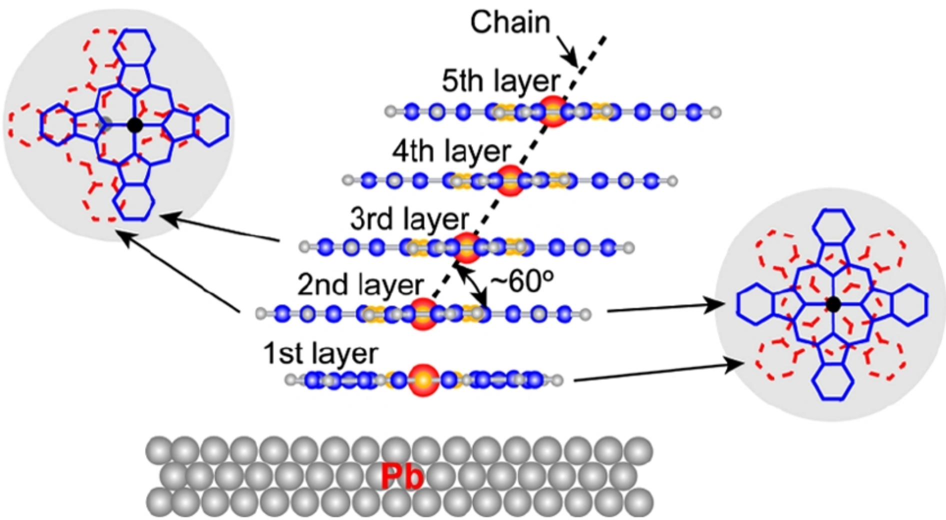
You want to achieve quantum coherence!



Desperately needed!

Friedman group: Phys. Rev. Research **2**, 032037(R) (2020)

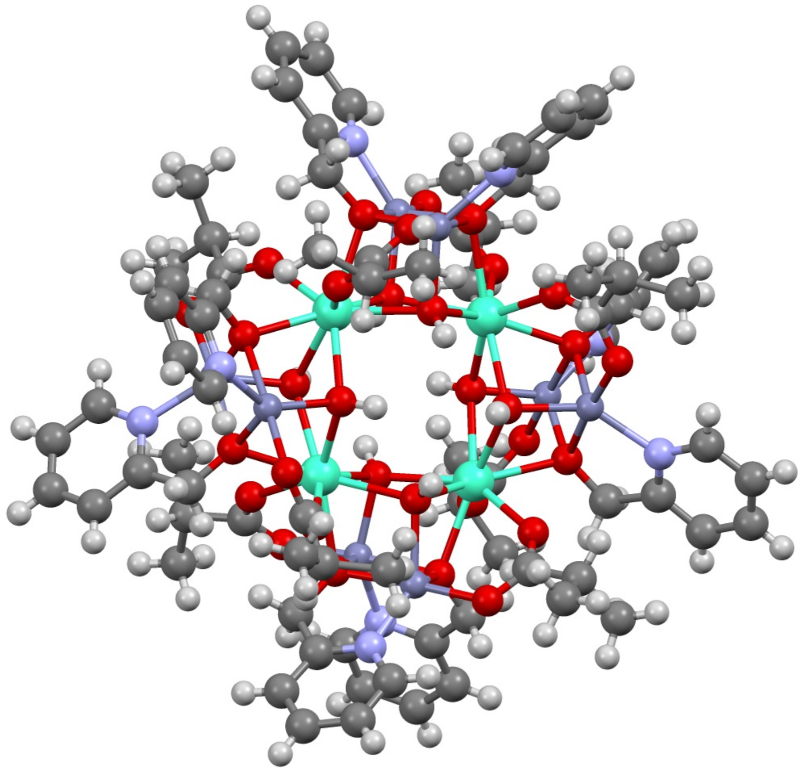
You want to deposit your molecule!



Next generation magnetic storage!

Xue group: Phys. Rev. Lett. **101**, 197208 (2008)

You want molecular magnetocalorics!



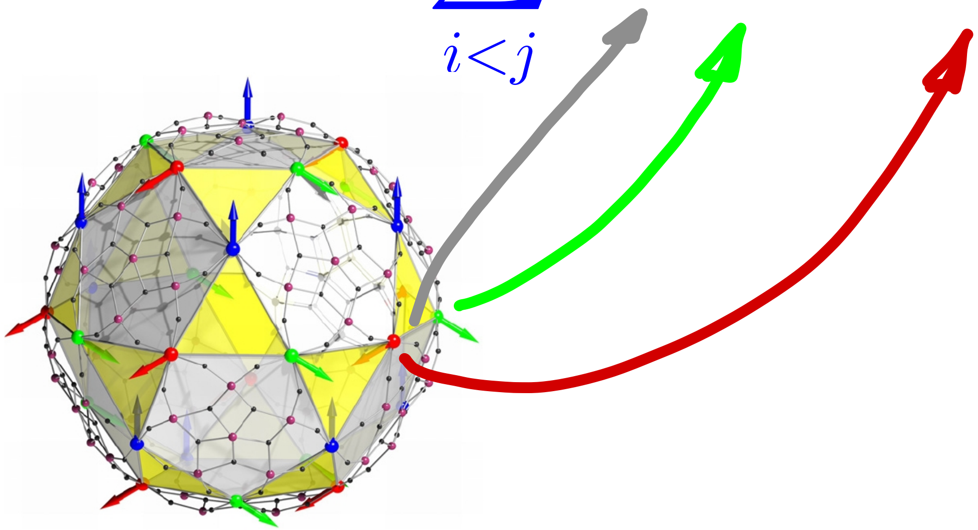
Cool!

Brechin group: Angew. Chem. Int. Ed. **51**, 4633 (2012)

You have got an idea about the modeling!

Heisenberg Zeeman

$$\underset{\sim}{H} = -2 \sum_{i<j} J_{ij}\, \underset{\sim}{\vec{s}}(i) \cdot \underset{\sim}{\vec{s}}(j) + g\, \mu_B\, B \sum_{i}^{N} \underset{\sim}{s}_z(i)$$



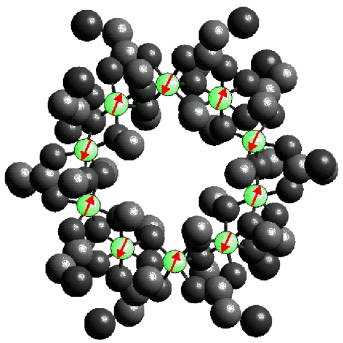
You have to solve the Schrödinger equation!

$$\underset{\sim}{H} \,|\, \phi_n \,\rangle \;=\; E_n \,|\, \phi_n \,\rangle$$

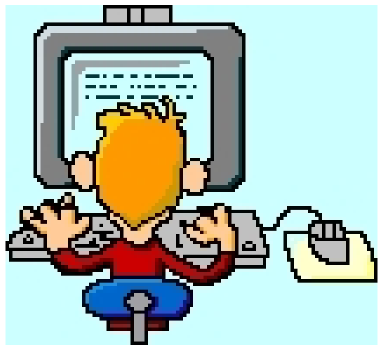
Eigenvalues E_n and eigenvectors $|\,\phi_n\,\rangle$

- needed for spectroscopy (EPR, INS, NMR);
- needed for thermodynamic functions (magnetization, susceptibility, heat capacity);
- needed for time evolution (pulsed EPR, simulate quantum computing, thermalization).

In the end it's always a big matrix!



$$\Rightarrow \begin{pmatrix} -27.8 & 3.46 & 0.18 & \cdots \\ 3.46 & -2.35 & -1.7 & \cdots \\ 0.18 & -1.7 & 5.64 & \cdots \\ \vdots & \vdots & \vdots & \cdots \end{pmatrix} \Rightarrow$$



Fe$^{\text{III}}_{10}$: $N = 10$, $s = 5/2$, dim$(\mathcal{H}) = (2s+1)^N$

Dimension=**60,466,176**. Maybe too big?

Can we evaluate the partition function

$$Z(T,B) = \mathrm{tr}\left(\exp\left[-\beta \underset{\sim}{H}\right]\right)$$

without diagonalizing the Hamiltonian?

Yes, with mathematical magic!

Typicality approach to molecular magnetism

Finite-temperature Lanczos method

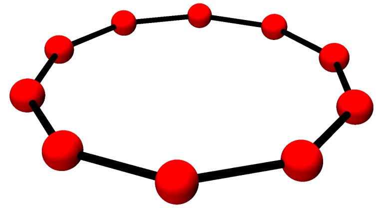
$$Z^{\text{FTLM}}(T,B) \quad \approx \quad \frac{1}{R}\sum_{r=1}^{R}\sum_{n=1}^{N_L} e^{-\beta\epsilon_n^{(r)}} |\langle\, n(r)\,|\, r\,\rangle|^2$$

- Idea 1: Trace estimation with random vectors.
  Idea 2: Spectral representation of $\exp\{-\beta \underset{\sim}{H}\}$ in Krylov space.

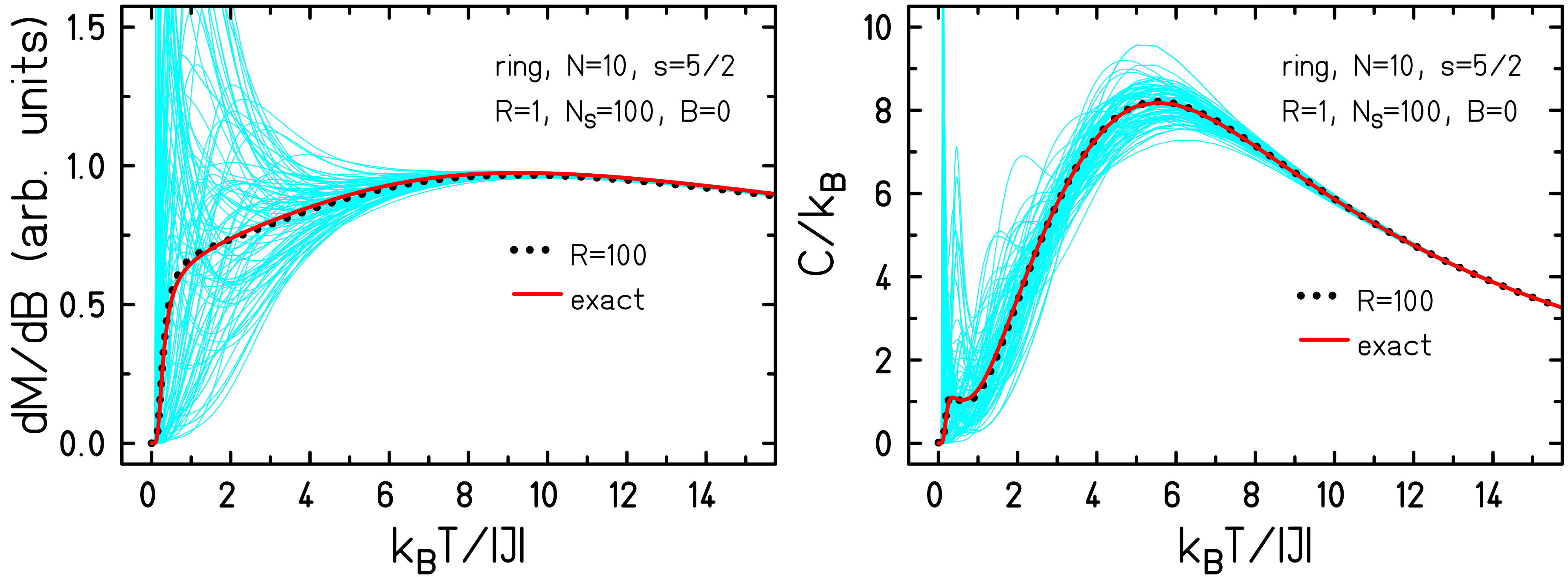
- Use symmetries!

- Partition function replaced by a small sum: $R = 1\dots100, N_L \approx 100$.

J. Jaklic and P. Prelovsek, Phys. Rev. B **49**, 5065 (1994).



FTLM 1: ferric wheel



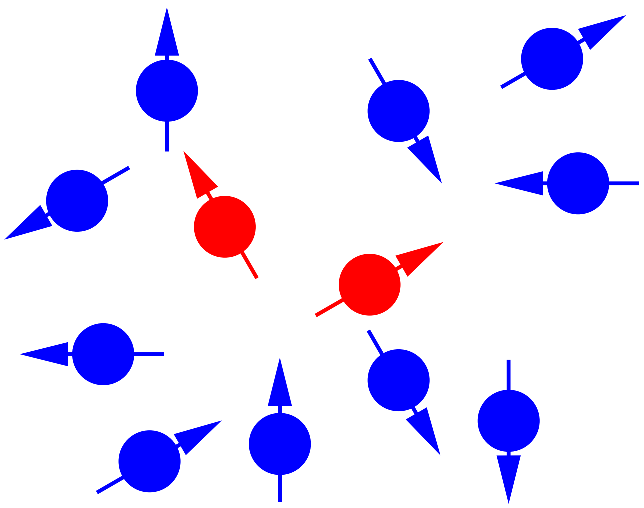
(1) J. Schnack, J. Richter, R. Steinigeweg, Phys. Rev. Research **2**, 013186 (2020).

(2) SU(2) & D_2: R. Schnalle and J. Schnack, Int. Rev. Phys. Chem. **29**, 403 (2010).

(3) SU(2) & C_N: T. Heitmann, J. Schnack, Phys. Rev. B **99**, 134405 (2019)

Studies on decoherence

Context

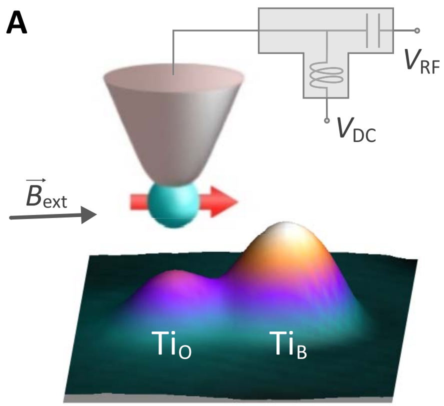


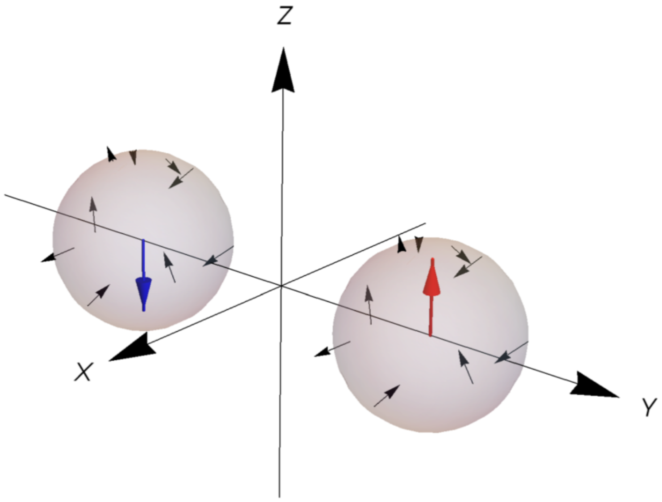
Investigation of decoherence of a subsystem if the combined system (including bath) is evolved via the time-dependent Schrödinger equation.

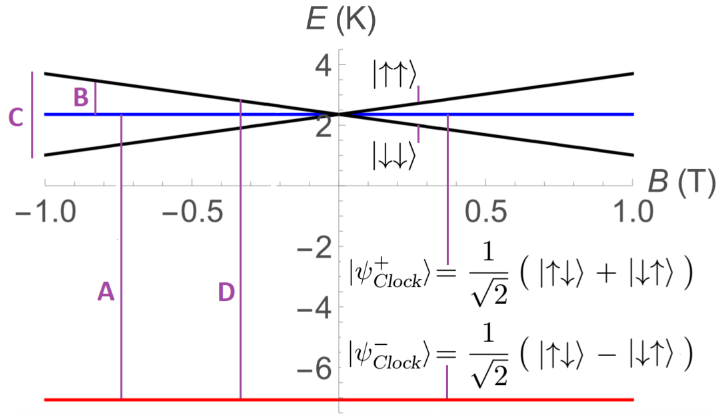
Employed measure of decoherence: reduced density matrix

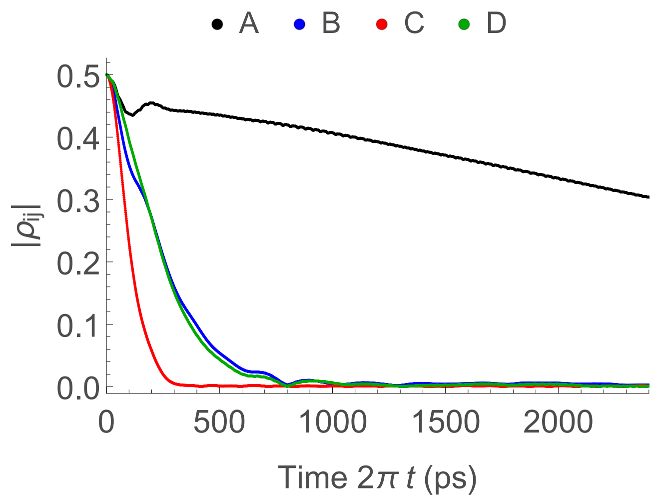
$$\underset{\sim}{\rho}_{\text{system}} = \text{Tr}_{\text{bath}}\left(\underset{\sim}{\rho}\right) , \quad \underset{\sim}{\rho} = |\,\Psi(t)\,\rangle\langle\,\Psi(t)\,|$$

Typicality: unitary-time evolution of pure state approximates dynamics in environment.







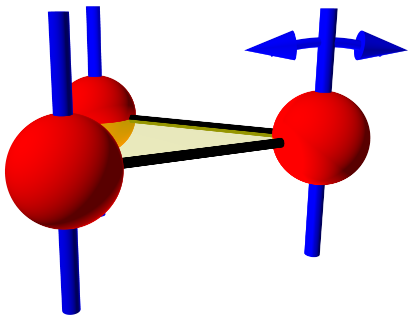


P. Vorndamme, J. Schnack, Phys. Rev. B 101, 075101 (2020)

Y. Bae, K. Yang, P. Willke, T. Choi, A. J. Heinrich, and C. P. Lutz, Sci. Adv. 4, eaau4159 (2018)

Spin-phonon interaction

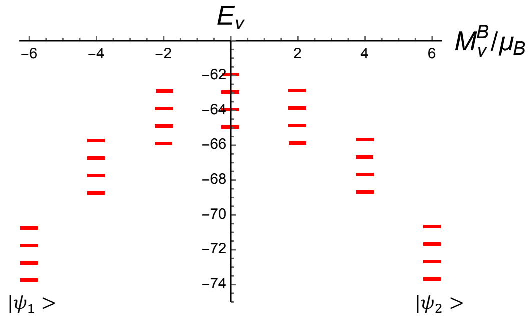
Spin-phonon interaction – our question



Can phonons induce a tunnel splitting?

Know that non-collinear easy axes produce tunnel splitting

Set up special phonon modes that tilt easy axes in plane with C_3 axis out of uniaxial alignment



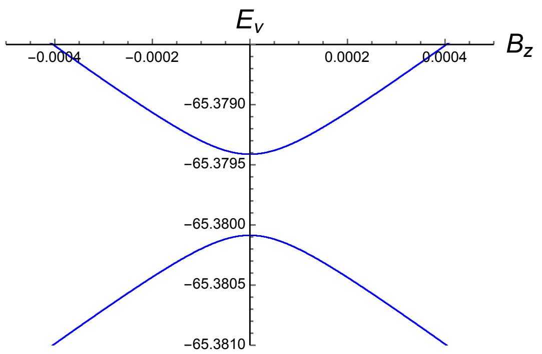
ADVANTAGE: quantum many-body solution for spins and phonons

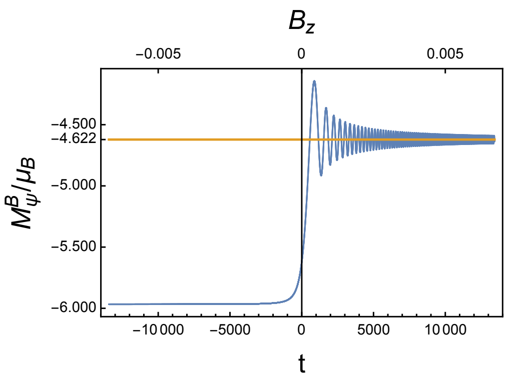
$\Rightarrow$ correlated spin-phonon states:

$$\Psi_\nu = \sum c^\nu_{m_1,m_2,m_3,n_1,n_2,n_3} \,|\, m_1, m_2, m_3, n_1, n_2, n_3 \,\rangle$$

(1) K. Irländer and J. Schnack, Phys. Rev. B **102**, 054407 (2020).

Spin-phonon interaction – our result (applies to integer spins)





Can phonons induce a tunnel splitting?

⇒ Yes, they can!

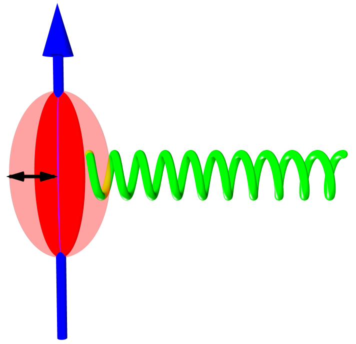
Ground state, practically, does not contain any phonons, nevertheless tunneling occurs. Coupling to zero-point motion suffices (2).

BAD NEWS: It is not enough to cool quantum devices, you have to prevent the coupling to disturbing sources at all.

Side remark: result probably already known in field of vibronic coupling (Atanasov, Shrivastava, Tsukerblat, Coronado).

(1) K. Irländer and J. Schnack, Phys. Rev. B **102**, 054407 (2020).
(2) F. Ortu *et al.*, Dalton Trans. **48**, 8541 (2019).

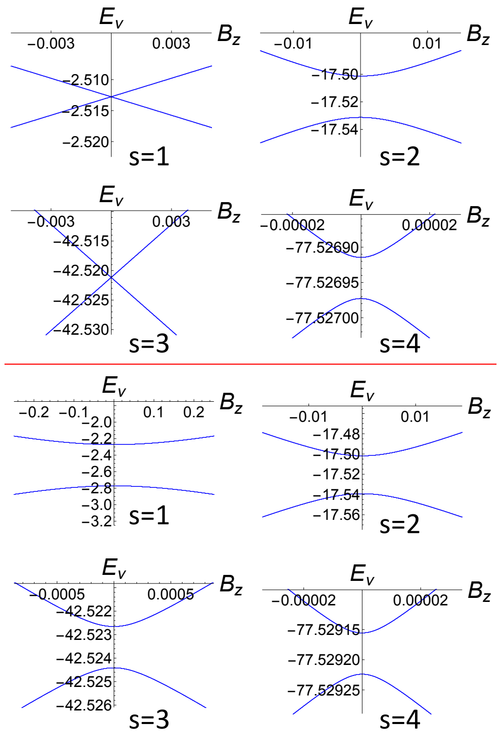
SUSY spin-phonon interaction (applies to integer spins)



$$\underset{\sim}{H} = D(\underset{\sim}{s}^z)^2 + E\left\{(\underset{\sim}{s}^x)^2 - (\underset{\sim}{s}^y)^2\right\} + g\mu_B B \underset{\sim}{s}^z + \underset{\sim}{H}_{\text{HO}}$$

Special phonons that modify only:

L: $E = \alpha\left(\underset{\sim}{a}^\dagger + \underset{\sim}{a}\right)$ or Q: $E = \alpha\left(\underset{\sim}{a}^\dagger + \underset{\sim}{a}\right)^2$



L: tunneling gap for even s, no gap for odd s.

This is not Kramers, but related to another symmetry.

Q: tunneling gap for all s.

RESULT: very interesting behavior; there are some phonons that do not produce a tunneling gap thanks to the way they couple. SUSY at work.

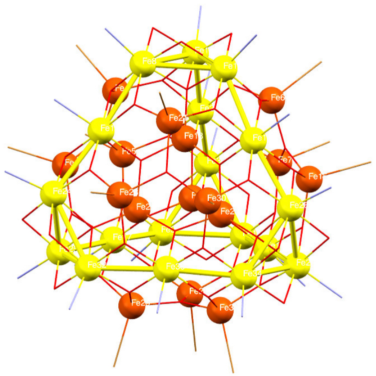
(1) K. Irländer, H.-J. Schmidt, J. Schnack, Eur. Phys. J. B **94**, 68 (2021)

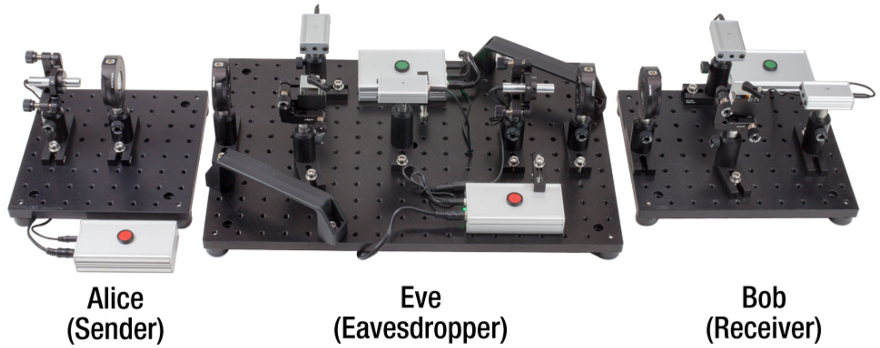
Examensarbeiten

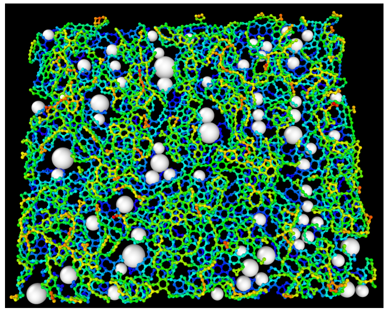
Einige Examensarbeiten 2013 – 2020

- Superheavies; Spektralfunktionen; Äqulibrierung;
- Dzyaloshinskii-Moriya; FTLM; Qubits; Magnetokalorik;
- Asymmetrischer Austausch; Symmetrien; Klassische Molekulardynamik.

Mögliche Themen

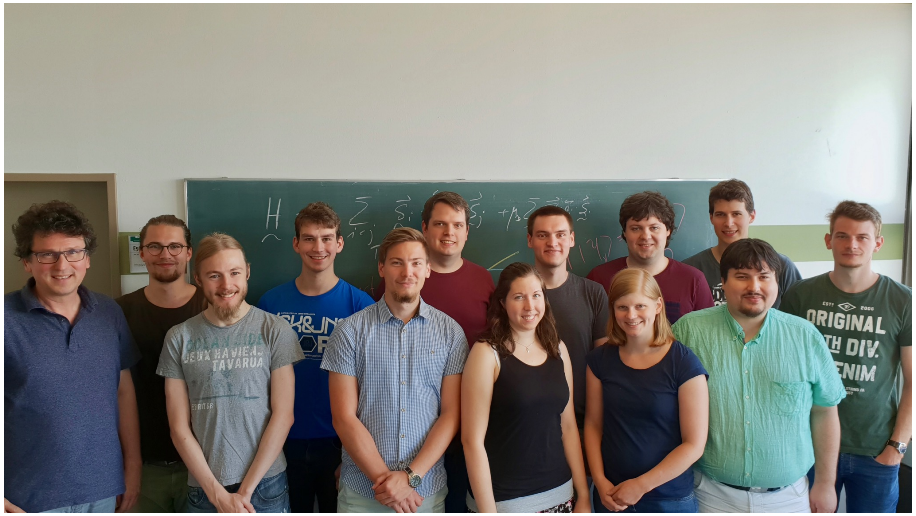


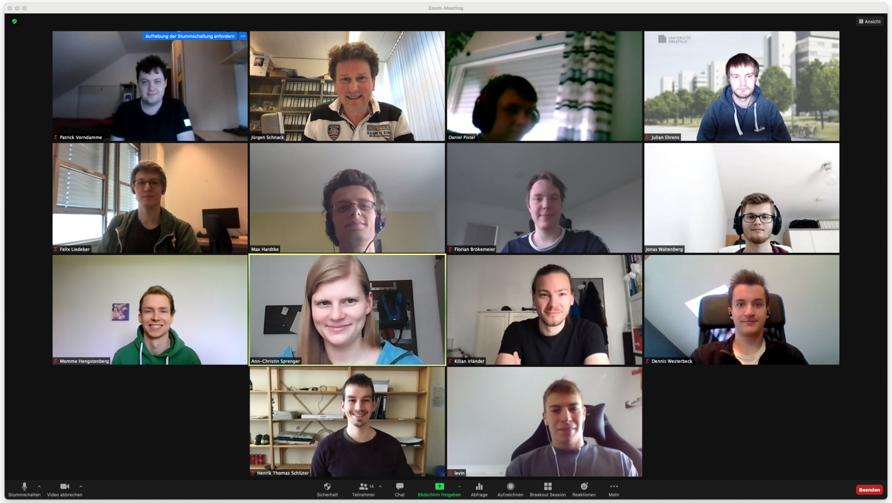


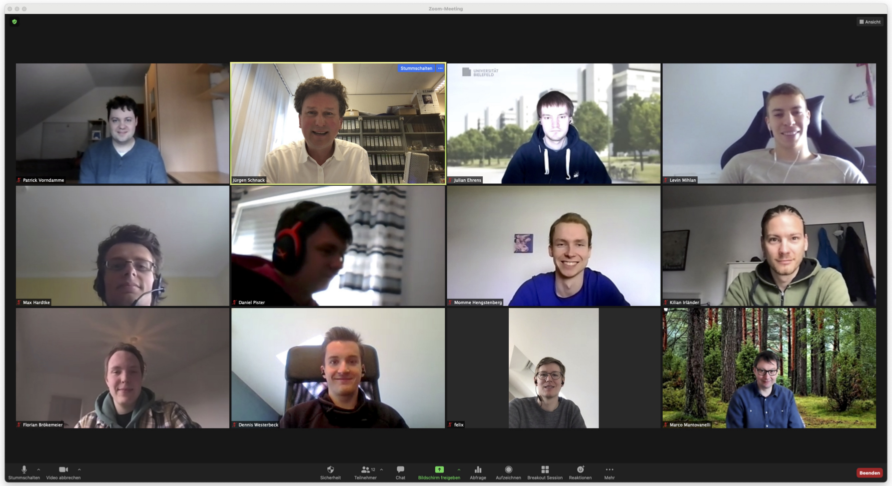


- Quantenspinringe mit dipolarer Wechselwirkung;
- Magnetokalorische Untersuchungen am quantenkritischen Punkt;
- Quantenkryptographie-Kit (Lehramt, Master);
- Spin-Phonon-Wechselwirkungen;
- Modellierung von Kohlenstoffnanomembranen.

Willkommen auf E5







Thank you very much for your attention.

The end.

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Highlights. Tutorials. Who is who. Conferences.