The epistemological power of spin systems*

Jürgen Schnack

Department of Physics – University of Bielefeld – Germany

http://obelix.physik.uni-bielefeld.de/∼schnack/

Seminar

Parma, Italy, 29 May 2024

* or better: What I learnt from spin systems.

UNIVERSITÄT BIELEFELD

Fakultät für Physik

DFG

lrz

You want to model a

many-body quantum system,

where the units have got m (relevant) levels?

Map it onto a spin system!

$$(m = 2s + 1)$$

. . . o.k., it's simplified, but often this will be a reasonable approach.

(The Ising model is used for nearly everything!)

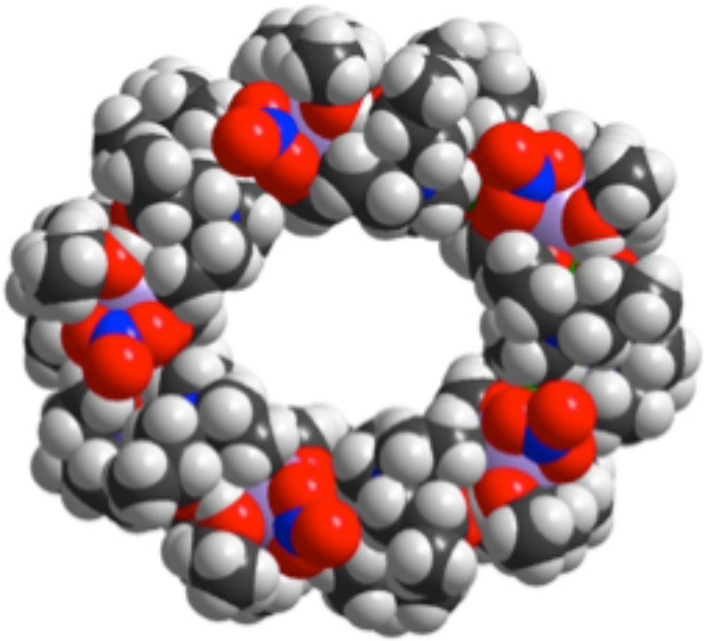
From the perspective of a bird's eye

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

1. Quantum magnetism
2. Random vector machinery
3. Foundations of thermodynamics
4. Quantum computing

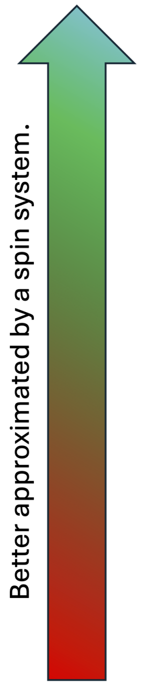
We are the sledgehammer team of matrix diagonalization.
Please send inquiries to jschnack@uni-bielefeld.de!

Quantum Magnetism



Quantum magnetism – a biased introduction

Magnetism = super rich = complicated!

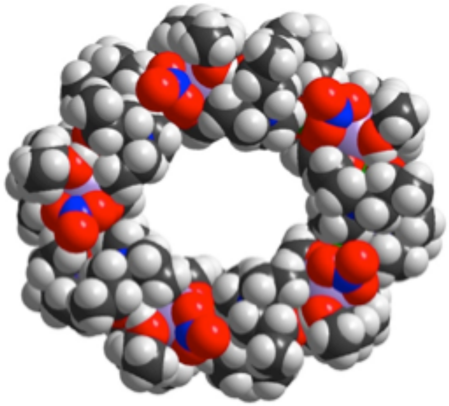


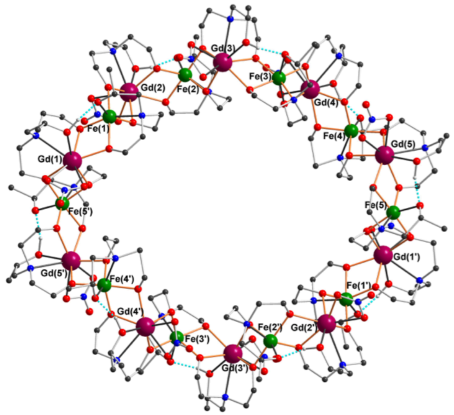
- Insulators, localized moments, small spin-orbit interaction; some iron group ions;
- Insulators, localized moments, spin-orbit interaction; e.g., single-ion anisotropy; molecular magnetism;
- Insulators, localized moments, strong spin-orbit interaction; e.g., effective doublets; Kitaev magnetism; single-ion magnets; toroidics;
- Conducting materials, topological insulators, altermagnets, ...

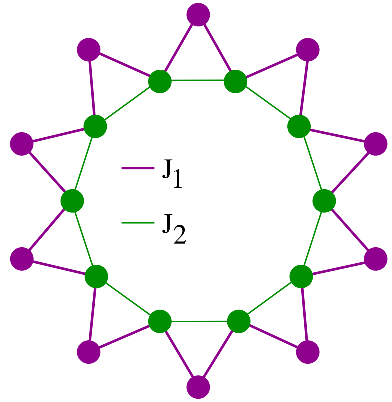
$\Rightarrow$ What we get: just magnets, magnetic storage, frustrated magnets, spin liquids, spin ice, quantum phase transitions, magnetocalorics, . . .

$Gd_{10}Fe_{10}$ – one example for quantum magnetism

Reduction + modelling.





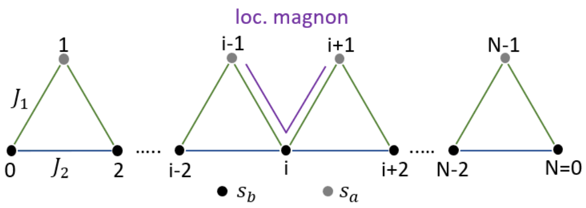


green: Fe ($s = 5/2$), purple: Gd ($s = 7/2$)

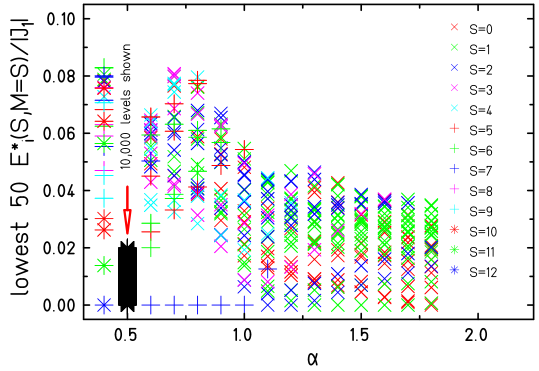
$$\underset{\sim}{H} = -2 \sum_{i<j} J_{ij} \, \underset{\sim}{\vec{s}}_i \cdot \underset{\sim}{\vec{s}}_j + g \, \mu_B \, B \sum_{i}^{N} \underset{\sim}{s}_i^z$$

A. Baniodeh *et al., npj Quantum Materials **3**, 10 (2018)*

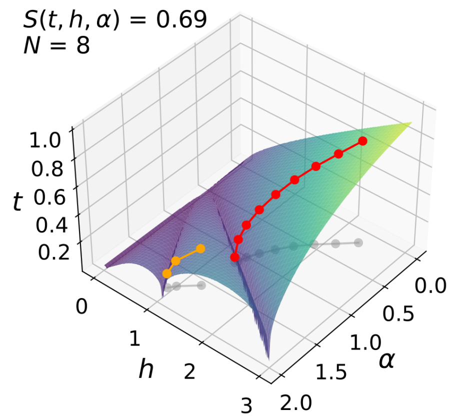
$Gd_{10}Fe_{10}$ – intermezzo: delta chain $s = 1/2$



frustrated structure



quantum phase transition



magneto- and barocaloric

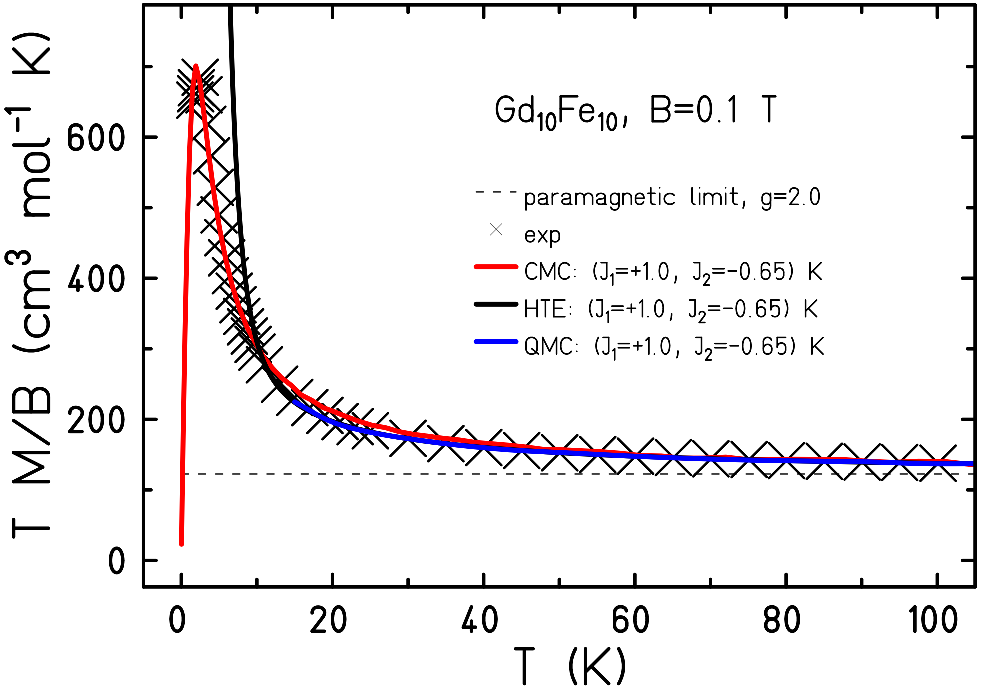
$\alpha = |J_2/J_1|$

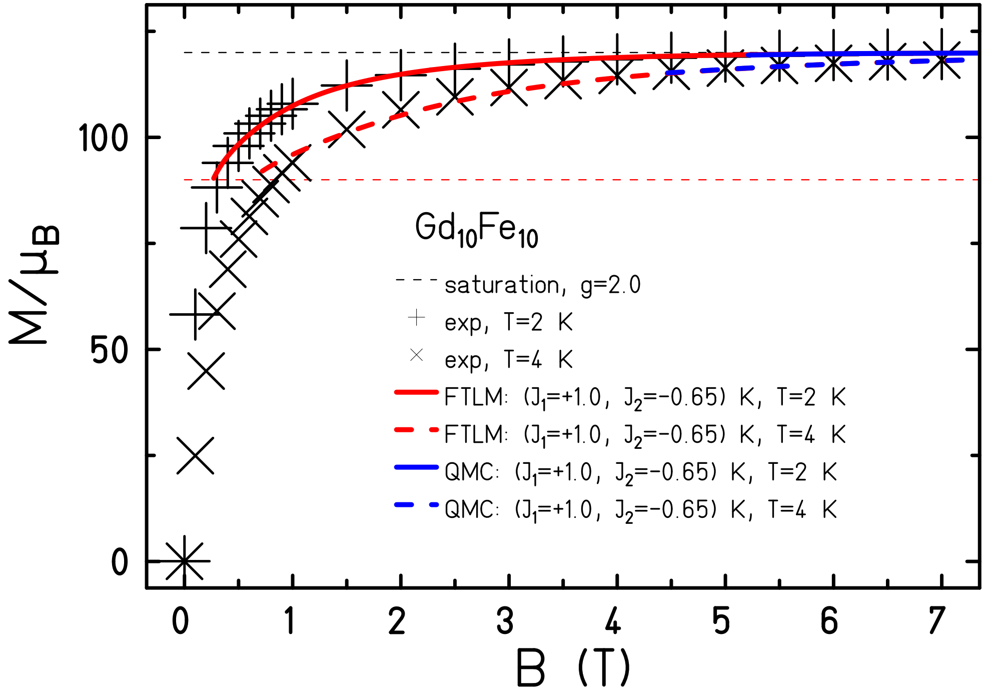
$t = k_B T/|J_1|, h = g\mu_B B/|J_1|$

Magneto- and barocaloric allow to heat and cool via changes of magnetic field and pressure.

N. Reichert, H. Schlüter, T. Heitmann, J. Richter, R. Rausch, and J. Schnack, Z. Naturforsch. A **79**, 283 (2024).

$Gd_{10}Fe_{10}$ – fit of the model to observables





$\Rightarrow J_1 = 1.0$ K, $J_2 = -0.65$ K

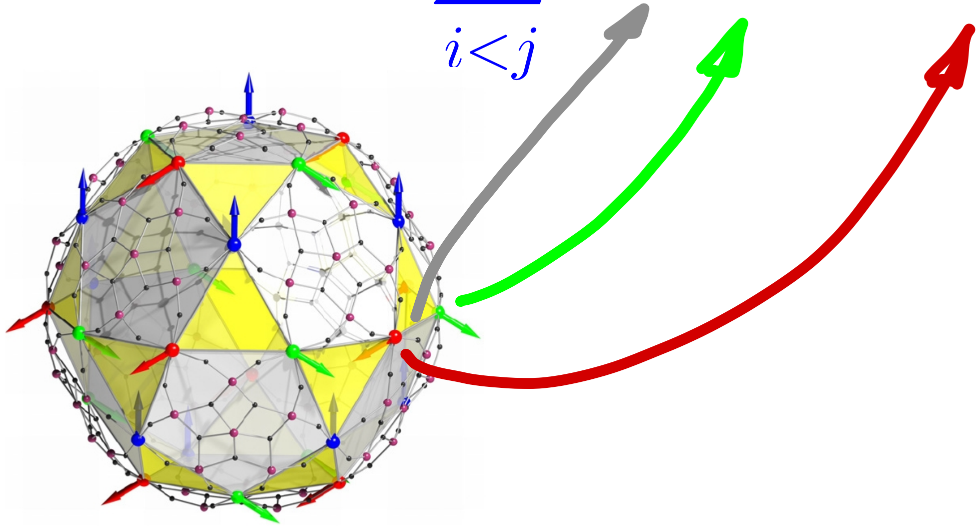
STOP: DIDN'T YOU HUSH UP SOMETHING???

Random Vector Machinery

We have got an idea about the modeling!

Heisenberg Zeeman

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



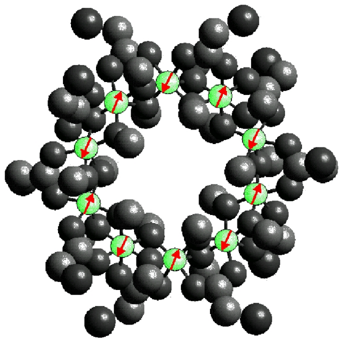
You have to solve the Schrödinger equation!

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

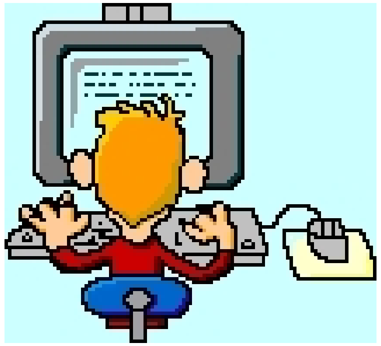
Eigenvalues E_n and eigenvectors $| \, \phi_n \, \rangle$

- 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!



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



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

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

Can we evaluate the partition function

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

without diagonalizing the Hamiltonian?

Yes, with magic!

Solution I: trace estimators

$$\text{tr}\left(\underset{\sim}{Q}\right) \approx \langle\, r \,|\, \underset{\sim}{Q} \,|\, r \,\rangle = \sum_{\nu} \langle\, \nu \,|\, \underset{\sim}{Q} \,|\, \nu \,\rangle + \sum_{\nu \neq \mu} r_\nu r_\mu \langle\, \nu \,|\, \underset{\sim}{Q} \,|\, \mu \,\rangle$$

$$|\, r \,\rangle = \sum_{\nu} r_\nu \,|\, \nu \,\rangle \,, \quad r_\nu = \pm 1$$

- $|\, \nu \,\rangle$ some orthonormal basis of your choice; not the eigenbasis of $\underset{\sim}{Q}$, since we don't know it.
- $r_\nu = \pm 1$ random, equally distributed. Rademacher vectors.
- Amazingly accurate, bigger (Hilbert space dimension) is better.

M. Hutchinson, Communications in Statistics - Simulation and Computation **18**, 1059 (1989).

Solution II: Krylov space representation

$$\exp\left[-\beta \underset{\sim}{H}\right] \approx \underset{\sim}{\mathbb{1}} - \beta \underset{\sim}{H} + \frac{\beta^2}{2!}\underset{\sim}{H}^2 - \dots \frac{\beta^{N_L-1}}{(N_L-1)!}\underset{\sim}{H}^{N_L-1}$$

applied to a state $|\, r\,\rangle$ yields a superposition of

$$\underset{\sim}{\mathbb{1}}\,|\, r\,\rangle, \quad \underset{\sim}{H}\,|\, r\,\rangle, \quad \underset{\sim}{H}^2\,|\, r\,\rangle, \quad \dots \underset{\sim}{H}^{N_L-1}\,|\, r\,\rangle \,.$$

These (linearly independent) vectors span a small space of dimension N_L;
it is called Krylov space.

Let's diagonalize $\underset{\sim}{H}$ in this space!

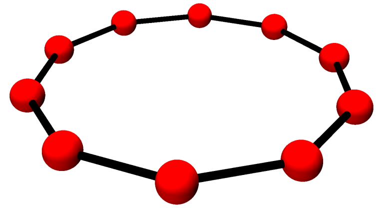
Partition function I: simple approximation

$$Z(T,B) \approx \langle\, r \,|\, e^{-\beta \underset{\sim}{H}} \,|\, r \,\rangle \approx \sum_{n=1}^{N_L} e^{-\beta \epsilon_n^{(r)}} |\langle\, n(r) \,|\, r \,\rangle|^2$$

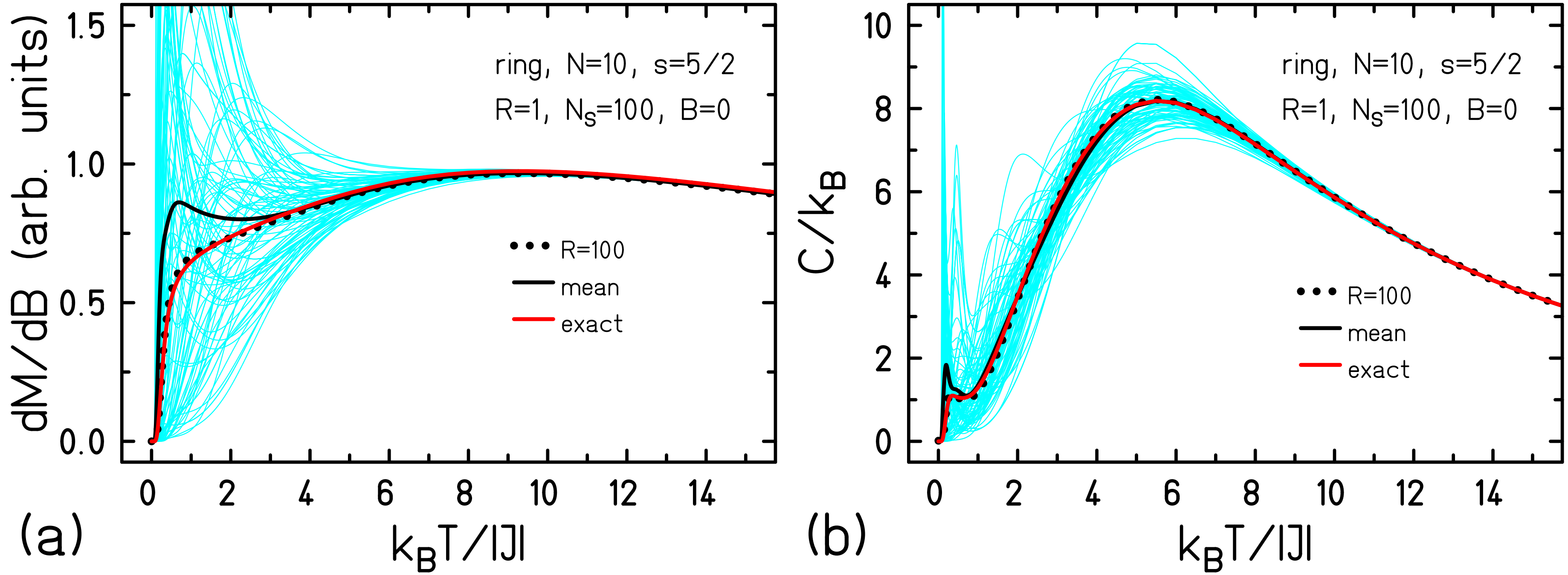
$$O^{\mathrm{r}}(T,B) \approx \frac{\langle\, r \,|\, \underset{\sim}{O} e^{-\beta \underset{\sim}{H}} \,|\, r \,\rangle}{\langle\, r \,|\, e^{-\beta \underset{\sim}{H}} \,|\, r \,\rangle} = \frac{\langle\, r \,|\, e^{-\beta \underset{\sim}{H}/2} \underset{\sim}{O} e^{-\beta \underset{\sim}{H}/2} \,|\, r \,\rangle}{\langle\, r \,|\, e^{-\beta \underset{\sim}{H}/2} e^{-\beta \underset{\sim}{H}/2} \,|\, r \,\rangle}$$

- Wow!!!
- One can replace a trace involving an intractable operator by an expectation value with respect to just ONE random vector evaluated by means of a Krylov space representation???
- Averaging over random vectors will improve the approximation.

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



FTLM 1: ferric wheel

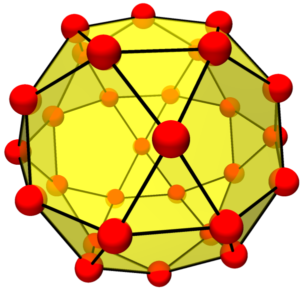


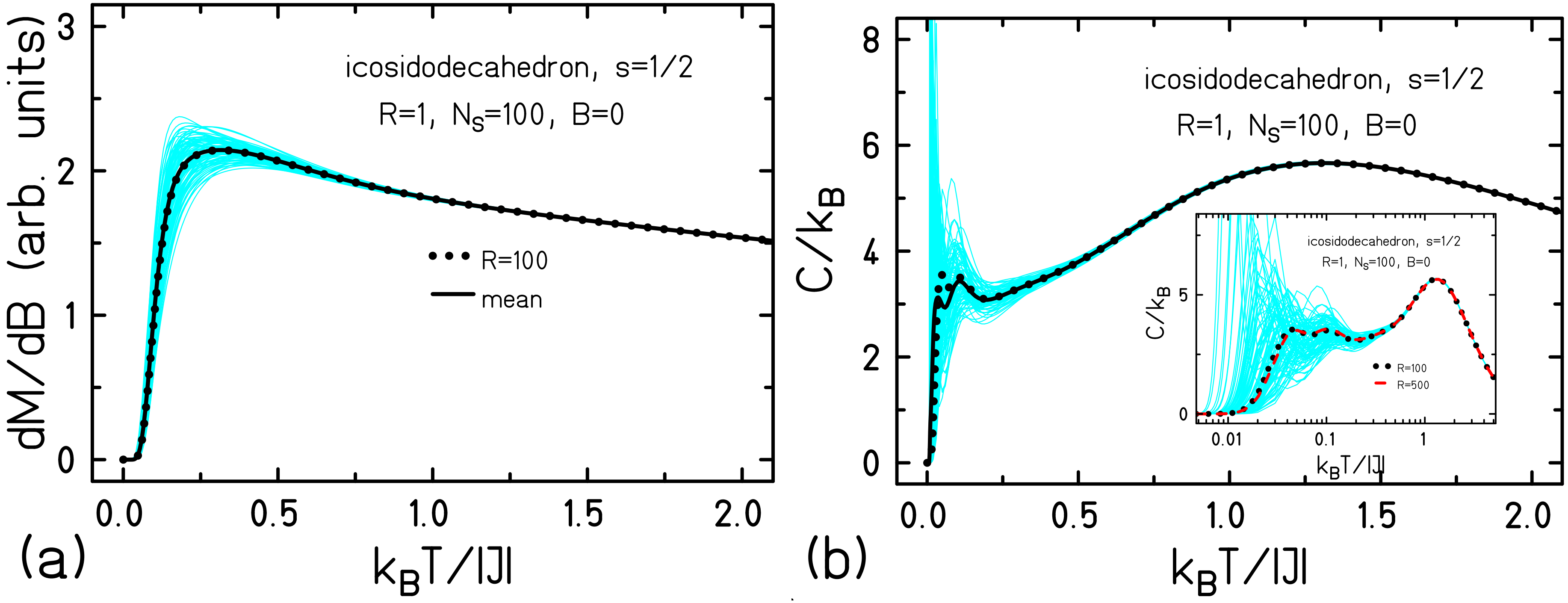
(1) J. Schnack, J. Richter, R. Steinigeweg, Phys. Rev. Research **2**, 013186 (2020).

(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)

FTLM 2: icosidodecahedron





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

(2) J. Schnack and O. Wendland, Eur. Phys. J. B **78**, 535 (2010).

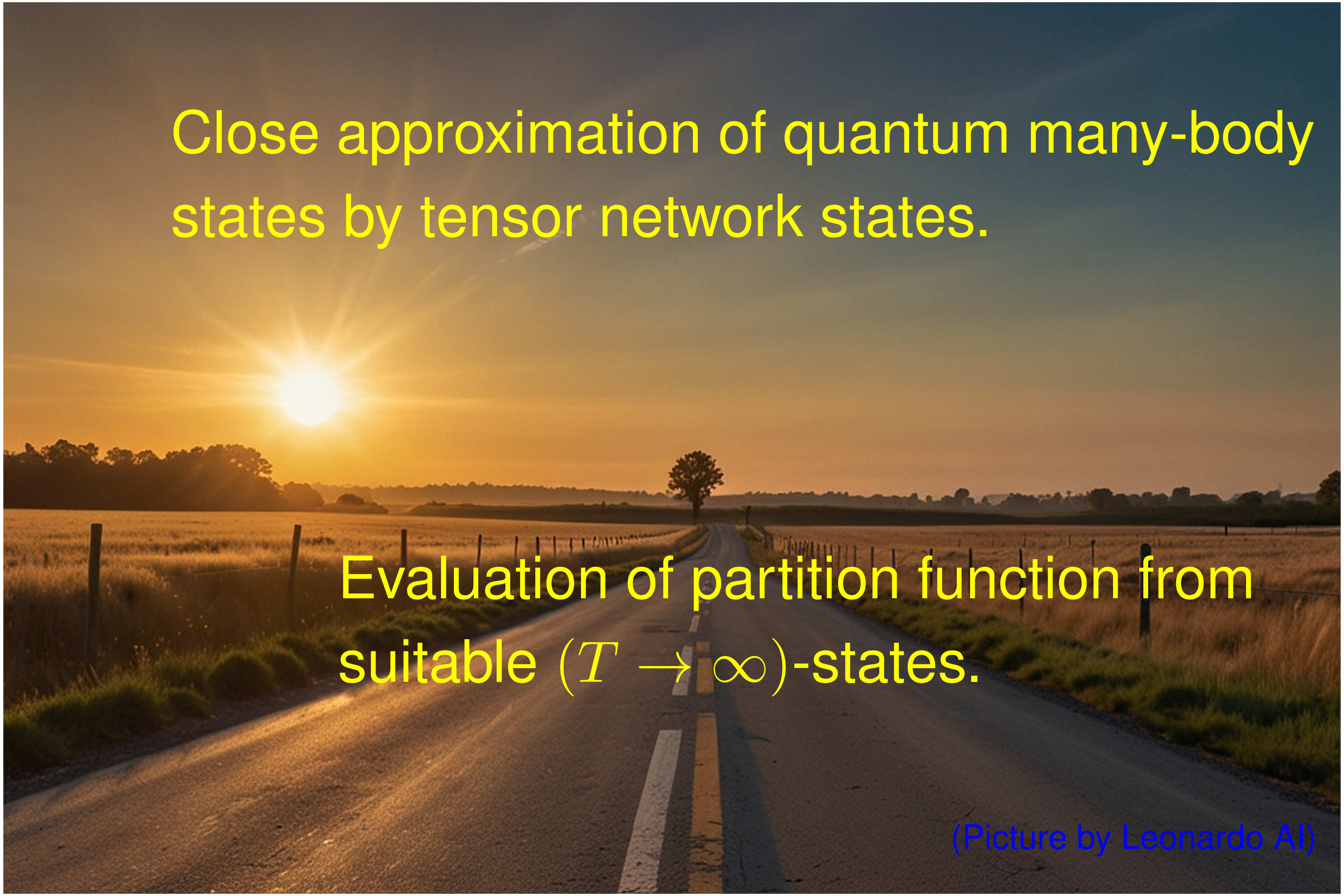
The greater picture

$$Z(T,B) \approx \langle\, r \,|\, e^{-\beta \underset{\sim}{H}} \,|\, r \,\rangle = \langle\, r \,|\, e^{-\frac{\beta}{2} \underset{\sim}{H}} \quad e^{-\frac{\beta}{2} \underset{\sim}{H}} \,|\, r \,\rangle$$

- This is an integration in imaginary time from $-it = 0$ to $-it = \beta/2$!
- Typicality = any random vector will do: $|\, r \,\rangle \equiv |\, T = \infty \,\rangle$
  This is not a thermal density matrix!
- Wow!!!

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

The future



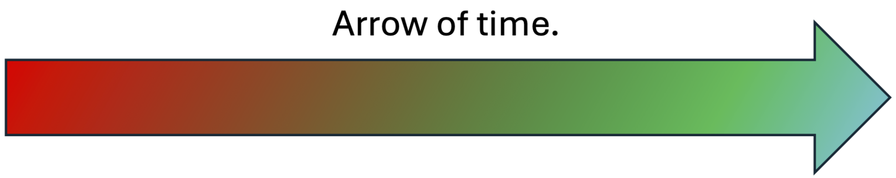
Close approximation of quantum many-body states by tensor network states.

Evaluation of partition function from suitable $(T \to \infty)$-states.

(Picture by Leonardo AI)

Foundations of Thermodynamics

Emergence of thermodynamics



Fundamental questions concerning thermodynamics

- How does thermodynamics follow from quantum mechanics?
- How does the 2nd law of thermodynamics emerge in view of time-reversal invariance of quantum mechanics and almost all fundamental laws?
- How do we understand equilibration/thermalization in closed systems?
- Closed system = no bath = unitary time evolution $\Rightarrow$ entropy constant! Thermalization?
- These questions are studied with the help of spin systems since we can do time evolution for rather large spin systems.

Deutsch, Srednicki, Goldstein, Lebowitz, Tumulka, Zanghi, Popescu, Short, Winter, Sugiura, Shimizu, Tasaki, Reimann, Gemmer, Steinigeweg, Eisert, Rigol, Santos, . . .

Typicality bill of rights – DFG research unit FOR 2692

“All” random states are equal(ly hot)

- A. Hams, H. De Raedt, Fast algorithm for finding the eigenvalue distribution of very large matrices, Phys. Rev. E 62, 4365 (2000)
- J. Schnack, J. Richter, R. Steinigeweg, Accuracy of the finite-temperature Lanczos method compared to simple typicality-based estimates, Phys. Rev. Research 2, 013186 (2020)

“All” non-equilibrium states relax equal

- C. Bartsch, J. Gemmer, Dynamical typicality of quantum expectation values, Phys. Rev. Lett., 102, 110403 (2009)
- P. Reimann, J. Gemmer, Why are macroscopic experiments reproducible? Imitating the behavior of an ensemble by single pure states, Physica A 552, 121840 (2020)
- T. Heitmann, J. Richter, D. Schubert, R. Steinigeweg, Selected applications of typicality to real-time dynamics of quantum many-body systems, Zeitschrift für Naturforschung A 75, 421 (2020)

“All” similar Hamiltonians produce equal time-evolution

- P. Reimann, Typical fast thermalization processes in closed many-body systems, Nat. Commun. 7, 10821 (2016)
- L. Dabelow, P. Reimann, Relaxation Theory for Perturbed Many-Body Quantum Systems versus Numerics and Experiment, Phys. Rev. Lett. 124, 120602 (2020)

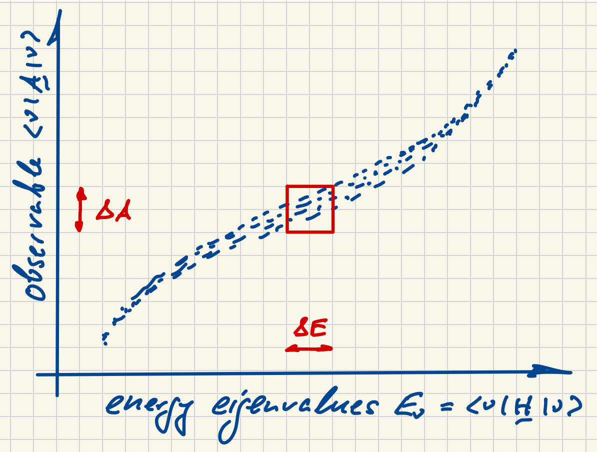
S. Lloyd@arXiv:1307.0378: Pure state quantum statistical mechanics and black holes, submitted to PRB in 1988 but rejected by one sentence referee report: “There is no physics.”
Deutsch, Srednicki, Goldstein, Lebowitz, Tumulka, Zanghi, Popescu, Short, Winter, Sugiura, Shimizu, . . .

One example – eigenstate thermalization hypothesis (ETH)

$$\langle\, \Psi(t) \,|\, \underset{\sim}{A} \,|\, \Psi(t) \,\rangle$$

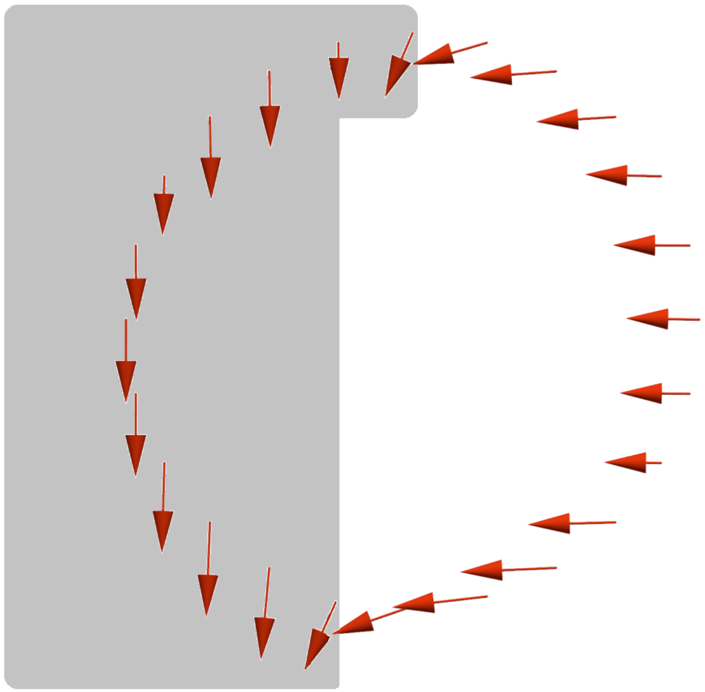
$$= \sum_{\mu,\nu} \langle\, \Psi(0) \,|\, \mu \,\rangle\langle\, \mu \,|\, \underset{\sim}{A} \,|\, \nu \,\rangle\langle\, \nu \,|\, \Psi(0) \,\rangle e^{i(E_\mu - E_\nu)t}$$

$$\approx \sum_{\nu} A_{\nu\nu} |\langle\, \nu \,|\, \Psi(0) \,\rangle|^2$$



- If $|\, \Psi(0) \,\rangle$ distributed across a small energy shell, all $A_{\nu\nu}$ assume the same value, and thus the expectation value is equal to the microcanonical value for almost all times.
- Such expectation values are indistinguishable from thermal values!

Second example - Guess what happens!



- System of N spins (e.g. $s = 1/2$);
- Heisenberg Hamitonian and magnetic field along z–direction;
- Unitary time evolution of many-body state;
- Initial state, e.g. product state or pre-quench state, with single spin expectation values in x–y–plane;
- **What do you expect?**
- $\Rightarrow$ Movie.

Synchronization – Technical details I

Heisenberg model: SU(2) invariant; simultaneous eigenstates $|\,\nu\,\rangle$ with

$$(\underset{\sim}{H}_0 + \omega_L \underset{\sim}{S}^z)\,|\,\nu\,\rangle = (E_\nu^{(0)} + \omega_L M_\nu)\,|\,\nu\,\rangle\ ,\ \underset{\sim}{\vec{S}}^2\,|\,\nu\,\rangle = S_\nu(S_\nu+1)\,|\,\nu\,\rangle\ ,\ \underset{\sim}{S}^z\,|\,\nu\,\rangle = M_\nu\,|\,\nu\,\rangle$$

For a general time evolution of an expectation value we obtain

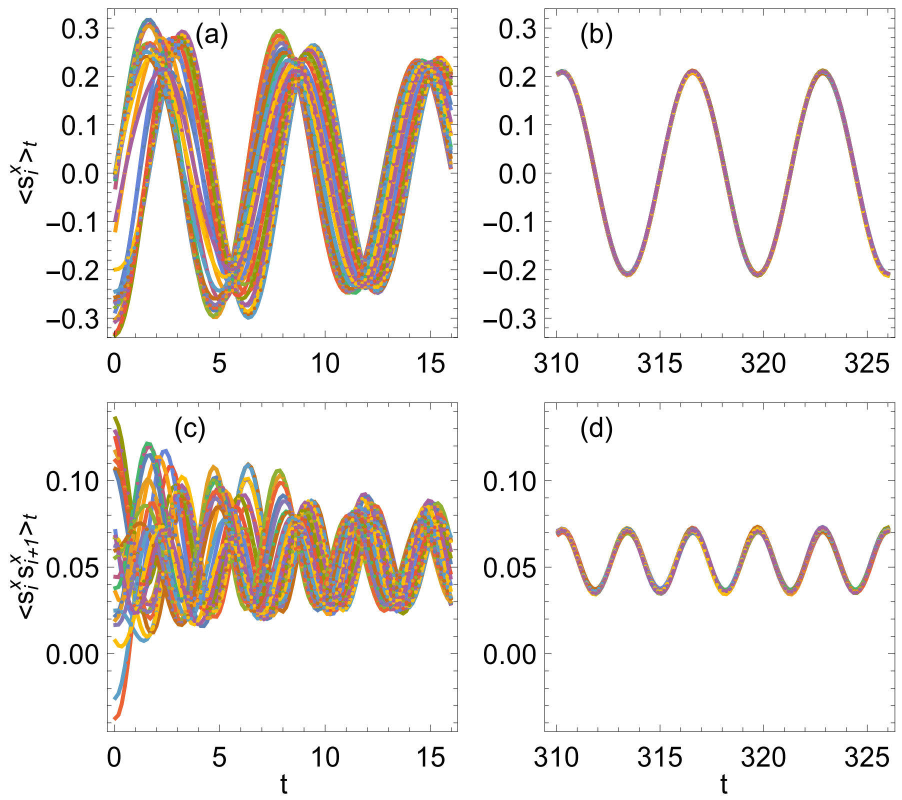
$$\langle\,\underset{\sim}{A}\,\rangle_t \quad := \quad \text{tr}\{\underset{\sim}{\rho}(t)\underset{\sim}{A}\} = \sum_{\mu,\nu} \rho_{\mu\nu} A_{\nu\mu}\, e^{i(E_\nu^0 - E_\mu^0 + [M_\nu - M_\mu]\omega_L)t} = \sum_{\Delta M} f_{\Delta M}(t)\, e^{i\Delta M \omega_L t}$$

$$\langle\,\underset{\sim}{A}\,\rangle_t \ \Rightarrow \ \sum_{\Delta M} \bar{f}_{\Delta M}\, e^{i\Delta M \omega_L t}$$

Equilibration of Fourier coefficients $\bar{f}_{\Delta M}$ can be shown under rather general assumptions (1).

(1) P. Reimann, P. Vorndamme, J. Schnack, *Non-equilibration, synchronization, and time crystals in isotropic Heisenberg models,* Phys. Rev. Research **5**, 043040 (2023)

Synchronization – homogeneous spin ring, $N = 24$

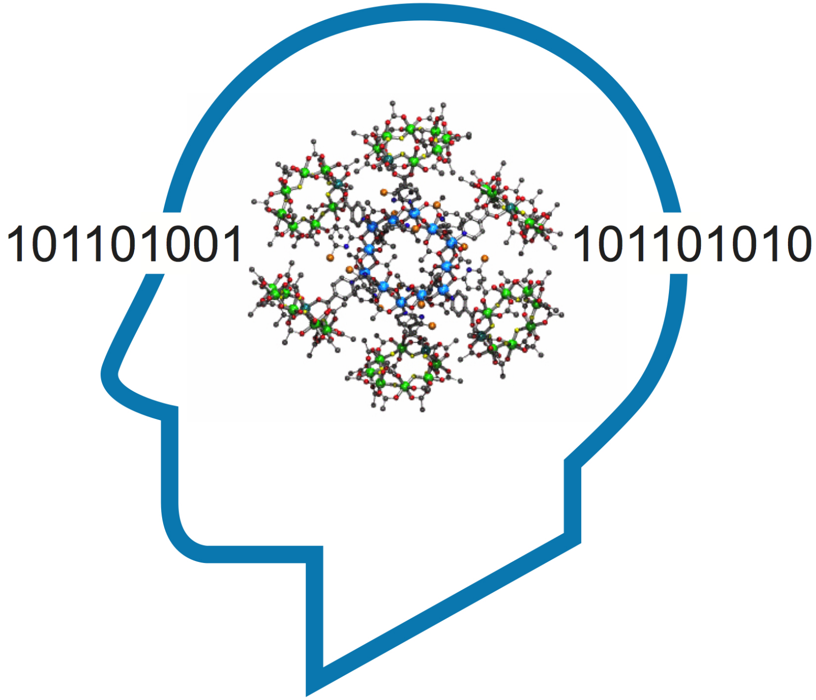


- $\underset{\sim}{s}_i^x \propto \left(\underset{\sim}{s}_i^+ + \underset{\sim}{s}_i^-\right)$
  thus $|\omega| = \omega_L$

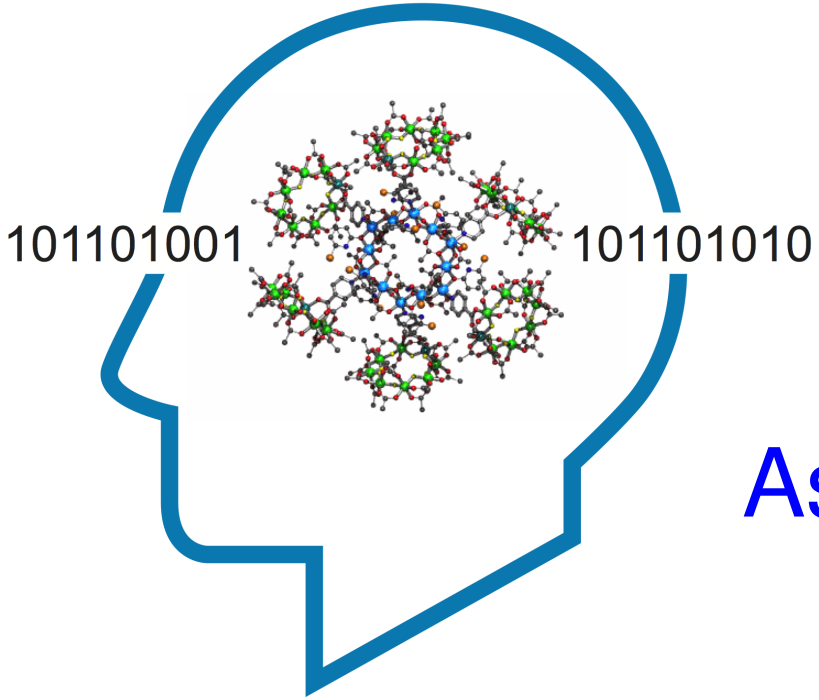
- $\underset{\sim}{s}_i^x \underset{\sim}{s}_{i+1}^x \propto \left(\underset{\sim}{s}_i^+ \underset{\sim}{s}_{i+1}^+ + \underset{\sim}{s}_i^+ \underset{\sim}{s}_{i+1}^- + \underset{\sim}{s}_i^- \underset{\sim}{s}_{i+1}^+ + \underset{\sim}{s}_i^- \underset{\sim}{s}_{i+1}^-\right)$
  thus $|\omega| = 2\omega_L$

P. Reimann, P. Vorndamme, J. Schnack, *Non-equilibration, synchronization, and time crystals in isotropic Heisenberg models,* Phys. Rev. Research **5**, 043040 (2023)

Quantum Computing



Quantum Computing



Ask the experts in Parma!

Summary

- Spin systems are very useful approximations in areas of many-body physics where the unit has got only limited options.

  However, . . .

- “If the only tool you have is a hammer, you tend to see every problem as a nail.”
  (Abraham Kaplan, 1964; Abraham Maslow, 1966)

Thank you very much for your attention.