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Quantifying quantum coherence in molecular magnetic systems

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List of Contents

Introduction

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- Miniaturization of electronic devices:
- Technological breakthrough;
- Quantum Computation:
  - Outperform classical computers;
  - Exploiting quantum properties
- Demand for the development of novel materials
  - Design and synthesis;
  - Characterization of its quantum properties;
- Molecular magnetic systems $\Rightarrow$ new quantum technologies.

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Quantum computing in molecular magnets

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Department of Physics and Astronomy, University of Basel, Klingelbergstrasse 82, 4056 Basel, Switzerland

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- Stability of its quantum properties;
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- Control the quantum properties;
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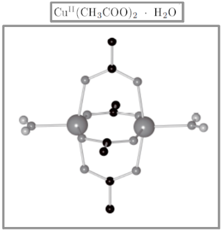
Low-Dimensional Molecular Magnetism

Introduction

- Brief History



Atomic structure of copper acetate dimer[1]

[1] BLEANEY, B.; BOWERS, K. D.; *Anomalous paramagnetism of copper acetate.* Proc. R. Soc. A, 212(1119): 451-465, 1952.

Main Properties and Fundamental Aspects

- Brief History
- Molecular magnetism

- Chemistry-Magnetism;
- Non-cooperative;
- Short range interaction;
- Located;
- Orbitals d, f, p;
- Low Dimensional;

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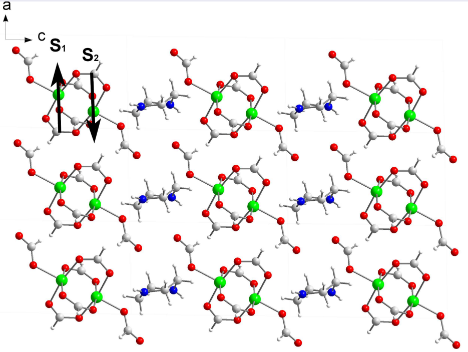
Low-Dimensional Molecular Magnetism

Geometric Configurations



Crystal structure of $Cu_2\ (HCOO)_4\ (HCOOH)_2\ (C_4H_{1}0N_2)$

Low-Dimensional Molecular Magnetism

Hamiltonians and Interactions:

- Heisenberg Hamiltonian:

$$\mathbf{H}_{hei} = -J\vec{S}_1 \cdot \vec{S}_2;$$

$J = E_{AP} - E_P$

  - J=0, there is no interaction ($E_{AP} = E_P$).
  - J>0, parallel alignment ($E_{AP} > E_P$)
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- Zeeman:

$$\mathbf{H}_z = \mu_B \vec{B} \cdot \mathfrak{g} \cdot \vec{S};$$

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Low-Dimensional Molecular Magnetism

Thermodynamic Quantities:

$$\mathcal{H} = -J\vec{S}_1 \cdot \vec{S}_2 - g\mu_B \vec{B} \cdot (\vec{S}_1 + \vec{S}_2)$$

$$\mathcal{E}_{s,m_s} = -\frac{1}{2}J\left[s(s+1) - s_1(s_1+1) - s_2(s_2+1)\right] - g\mu_B B m_s$$

where $|s_1 - s_2| \leq s \leq s_1 + s_2$; and $m_s = -s, \ldots, +s$.

$$Z(T,B) = \sum_i e^{-\beta \mathcal{E}_i}$$

$$F(T,B) = -k_B T ln(Z(B,T))$$

$$M(T,B) = -\frac{\partial}{\partial B} F(T,B)$$

$$\chi_{ij} = \lim_{B \to 0} \mu_0 \frac{dM_j}{dB_i} = \frac{2N(g\mu_B)^2}{k_B T} \frac{1}{3 + e^{-J/k_B T}}$$

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Low-Dimensional Molecular Magnetism

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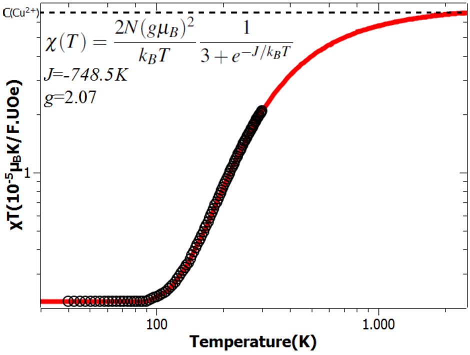

Quantum Coherence in Molecular Magnetic Systems

Quantum Entanglement

- Remarkable resource for quantum information processing;
- Let us consider the Hilbert space of a composite system:

$$\mathbb{H} = \mathbb{H}_1 \otimes \mathbb{H}_2 \otimes \cdots \otimes \mathbb{H}_n$$

- An entangled state can be defined as:

$$|\Psi\rangle \neq |\phi_1\rangle \otimes |\phi_2\rangle \otimes \cdots \otimes |\phi_n\rangle$$
$$\rho = \sum_i p_i \rho_1^{(i)} \otimes \rho_2^{(i)} \otimes \cdots \otimes \rho_n^{(i)}$$

- The best knowledge of a whole does not include the knowledge of its parts.

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Quantum Entanglement

- Let us consider the following example:

Event	Box A	Box B	Probability
1	0	1	50%
2	1	0	50%

$$|\phi_A\rangle = |\phi_B\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle + |1\rangle\right)$$

$$|\Psi\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle_A \otimes |1\rangle_B + |1\rangle_A \otimes |0\rangle_B\right) \neq |\phi_A\rangle \otimes |\phi_B\rangle \ .$$

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- Entangled $\Rightarrow$ Quantum Coherence + Classical Correlations;

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- Entangled states exhibit quantum and classical correlation,
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- Geometric approaches are widely used to characterize and quantify the quantum correlations.
- *Phys. Rev. Lett. 113, 140401 (2014)*:
  From the minimal distance $D(\rho, \sigma)$, between the quantum state ρ and a set $\{\sigma = \sum_k^d |k\rangle\langle k| \in \mathcal{I}\}$ of incoherent state.

$$\mathcal{C}_D = \min_{\{\sigma \in \mathcal{I}\}} D(\rho, \sigma)$$

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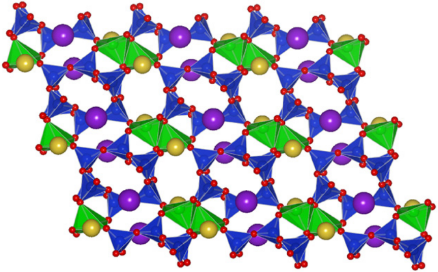
Results

Metal Silicate Framework $KNaCuSi_4O_{10}$



Crystal structure of the Metal Silicate Framework $KNaCuSi_4O_{10}$

Journal of Solid State Chemistry, 182(2), 253-258.

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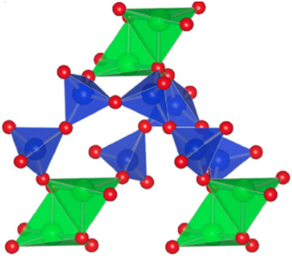

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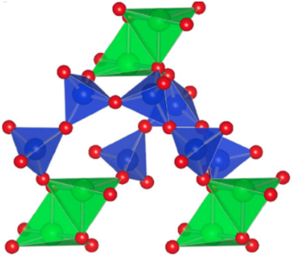

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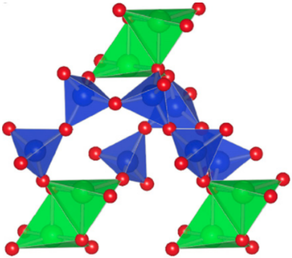

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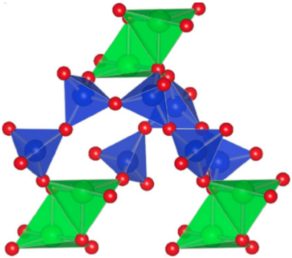

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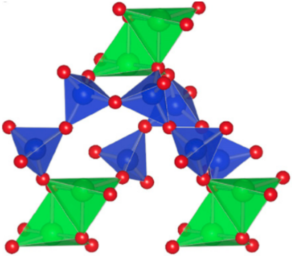

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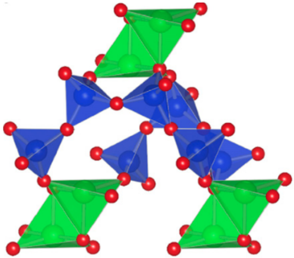

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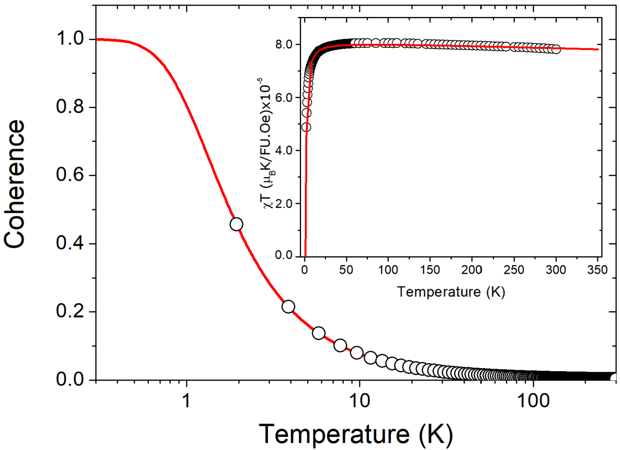

Acknowledgements: A.M. dos Santos - Oak Ridge National Laboratory, Tennessee USA

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- Kohn-Sham equations were solved;

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V_s(\vec{r})\right]\phi_i(\vec{r}) = E_i\phi_i(\vec{r})$$

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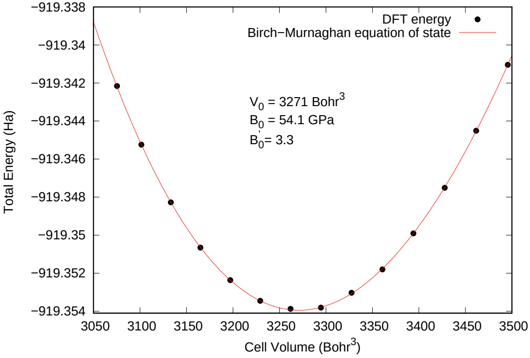
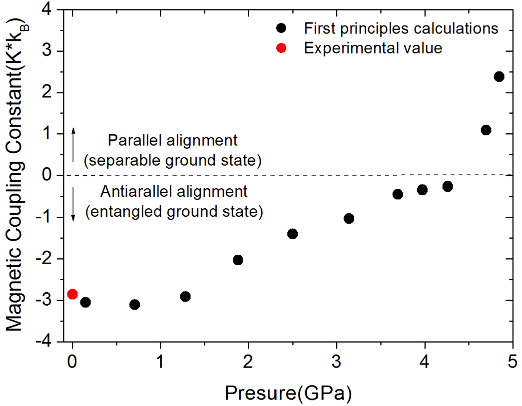
$$E(V) = E_0 + \frac{9V_0B_0}{16}\left\{\left[\left(\frac{V_0}{V}\right)^{\frac{2}{3}} - 1\right]^3 B_0' + \left[\left(\frac{V_0}{V}\right)^{\frac{2}{3}} - 1\right]^2 \left[6 - 4\left(\frac{V_0}{V}\right)^{\frac{2}{3}}\right]\right\}$$



Results

$$J = E_S - E_T$$



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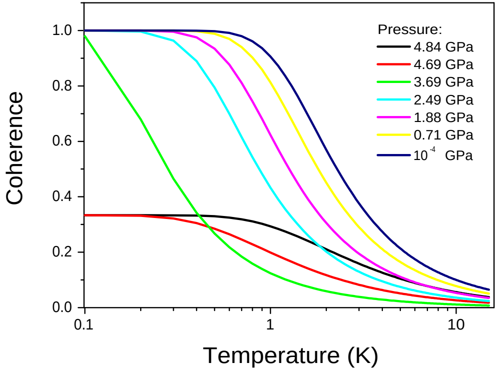


Temperature dependence of the quantum coherence calculated for different values of hydrostatic pressure.

Results

Influence of the longitudinal and transverse magnetic field

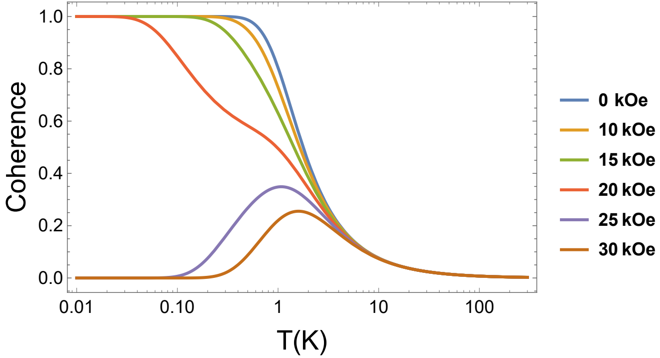
- Quantum coherence is basis dependent.
- Basis choice depends on the physical problem under investigation.
- Molecular magnetic systems: spin eigenbasis in a certain direction, $\{S_x, S_y, S_z\}$, within a quantum metrology setting.

The Hamiltonian model that rule this system interacting with an external magnetic field is given by:

$$\mathcal{H} = -J\vec{S}_1 \cdot \vec{S}_2 - \mu_B g \vec{B} \cdot \left(\vec{S}_1 + \vec{S}_1\right).$$

Longitudinal Magnetic Field

$$\mathcal{C}_z(T,B_z) = \left| \frac{1-e^{-4x}}{1+e^{-4x}+2\cosh(\beta h_z)} \right|$$



Longitudinal Magnetic Field

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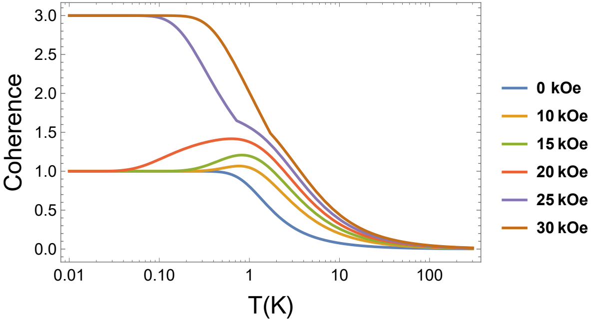
$$\mathcal{C}_x(T, B_x) = \frac{e^x}{Z}\left(\left|\cosh(\beta h_z) - 1\right| + 4\left|\sinh(\beta h_z)\right| + \left|\cosh(\beta h_z) - e^{-4x}\right|\right)$$



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That's all Folks!