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# Quantum entanglement in magnetic systems: theoretical aspects

1st eduQUTE school on quantum technologies

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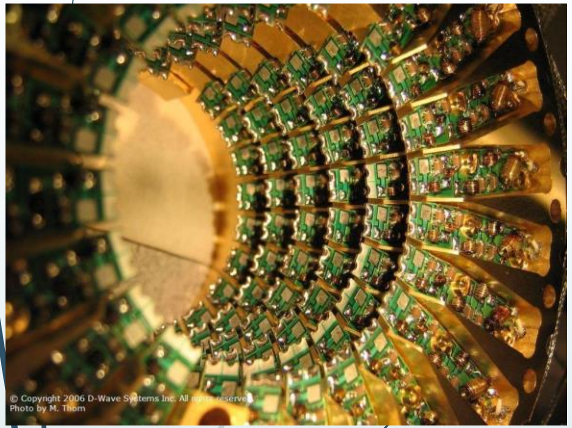
# Introduction and brief outline




## Quantum computation and quantum computer:

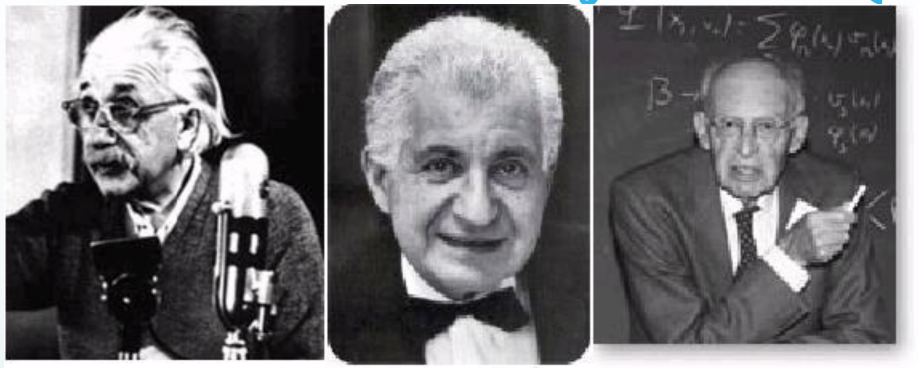
Quantum computer is a computational device, which makes direct use of quantum-mechanical phenomena such as quantum superposition and quantum entanglement, to perform logical operations with data.


## Quantum entanglement
## resource for quantum information processing

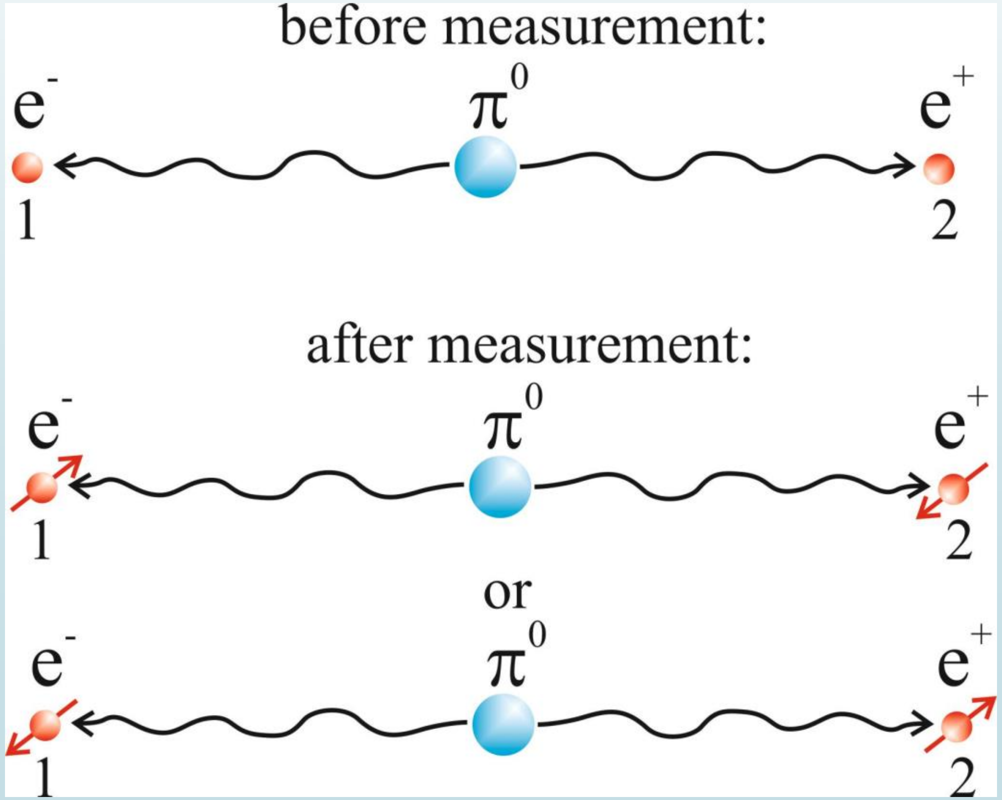
- What is quantum entanglement?
- How to characterize, define and quantify entanglement?
- How entanglement can be detected theoretically and experimentally?
- Entanglement between spins in magnetic systems…

# Quantum entanglement: historical perspectives

## Einstein-Podolsky-Rosen (EPR) paradox (Bohm version)



**Principle of locality**: measurement performed on one physical system should have no instantaneous effect upon another spatially separated physical system, because an influence cannot travel faster than the speed of light.




**entangled singlet**

$$|S\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\rangle_1|\downarrow\rangle_2 - |\downarrow\rangle_1|\uparrow\rangle_2\right)$$

**collapse - reduction**

$$|\mathrm{I}\rangle = |\uparrow\rangle_1|\downarrow\rangle_2$$

$$|\mathrm{II}\rangle = |\downarrow\rangle_1|\uparrow\rangle_2$$

**Entanglement:** measurements on spatially separated quantum systems instantaneously influence one another (Einstein's spooky action at distance).

# Quantum mechanics (QM) in a nutshell: pure and mixed states

Due to probabilistic character of QM, the experiment has to be repeated many times with an ensemble of copies of the same systems. When repeating experiment it might be difficult (or even impossible) to prepare the system in exactly the same state (or prepare perfectly identical copies), so that there is some uncertainty on the initial state.

$$|\psi\rangle = \sum_{j=1}^{n} c_j |\phi_j\rangle$$

$$\hat{A}|\phi_j\rangle = A_j |\phi_j\rangle$$

$$\hat{A}|\psi\rangle \Longrightarrow \begin{cases} |\phi_1\rangle, & |c_1|^2, & A_1 \\ \vdots & \vdots & \vdots \\ |\phi_j\rangle, & |c_j|^2, & A_j \\ \vdots & \vdots & \vdots \\ |\phi_n\rangle, & |c_n|^2, & A_n \end{cases}$$

Suppose that our information regarding the system is not complete. Let us associate the concept of state of a system with an ensemble of similarly prepared systems, which could have been prepared in principle but do not need to exist.

$$\langle \hat{A} \rangle = \langle \Psi | \hat{A} | \Psi \rangle \qquad \Longrightarrow \qquad \langle \hat{A} \rangle = \mathrm{Tr}(\hat{\rho}\hat{A})$$

$$\hat{\rho} = \sum_k p_k |\varphi_k\rangle\langle\varphi_k|$$

$\hat{\rho}$ - density operator or state operator or density matrix

**Pure state:** if a system can be described by a state vector $|\varphi\rangle$ and state operator $\hat{\rho} = |\varphi\rangle\langle\varphi|$

**Mixed state:** if a system cannot be described by a state vector $|\varphi\rangle$ and state operator $\hat{\rho} = |\varphi\rangle\langle\varphi|$

# Quantum superposition versus quantum entanglement or what entaglement is and what is not...

Two pure states for a couple of spin-1/2 particles:

$$|F\rangle = \frac{1}{2}\left(|\uparrow\rangle_1|\uparrow\rangle_2 - |\uparrow\rangle_1|\downarrow\rangle_2 - |\downarrow\rangle_1|\uparrow\rangle_2 + |\downarrow\rangle_1|\downarrow\rangle_2\right)$$

$$|S\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\rangle_1|\downarrow\rangle_2 - |\downarrow\rangle_1|\uparrow\rangle_2\right)$$

# Quantum superposition versus quantum entanglement or what entaglement is and what is not...

Two pure states for a couple of spin-1/2 particles:

$$\begin{aligned}|F\rangle &= \frac{1}{2}\left(|\uparrow\rangle_1|\uparrow\rangle_2 - |\uparrow\rangle_1|\downarrow\rangle_2 - |\downarrow\rangle_1|\uparrow\rangle_2 + |\downarrow\rangle_1|\downarrow\rangle_2\right)\\ &= \frac{1}{\sqrt{2}}\left(|\uparrow\rangle_1 - |\downarrow\rangle_1\right) \otimes \frac{1}{\sqrt{2}}\left(|\uparrow\rangle_2 - |\downarrow\rangle_2\right)\end{aligned}$$

**separable – quantum superposition**

$$\begin{aligned}|S\rangle &= \frac{1}{\sqrt{2}}\left(|\uparrow\rangle_1|\downarrow\rangle_2 - |\downarrow\rangle_1|\uparrow\rangle_2\right)\\ &\neq \left(a|\uparrow\rangle_1 + b|\downarrow\rangle_1\right) \otimes \left(c|\uparrow\rangle_2 + d|\downarrow\rangle_2\right)\end{aligned}$$

**nonseparable – quantum entanglement**

# Quantum entanglement: key features & definition

- nonlocality
- nonseparability

**A pure state is separable (entangled) if and only if it can (cannot) be factorized into a product of two pure states of both subsystems**

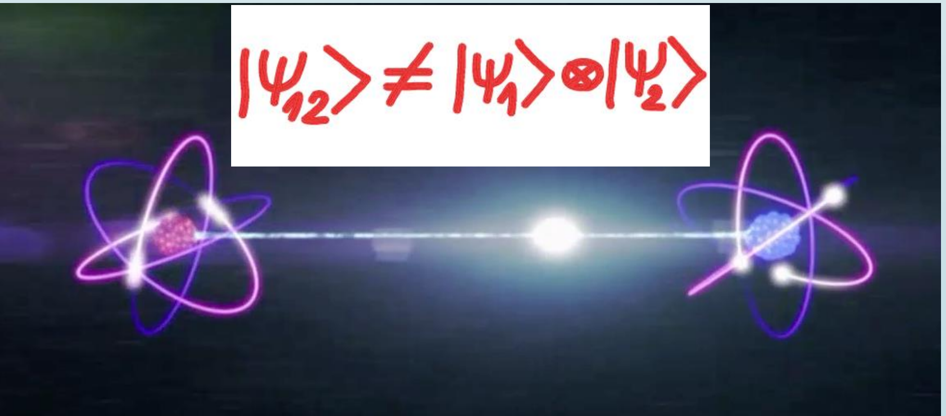
$$|\Psi_{12}\rangle = |\Psi_1\rangle \otimes |\Psi_2\rangle$$

$$|\Psi_{12}\rangle \in \mathcal{H}_{12} = \mathcal{H}_1 \otimes \mathcal{H}_2$$

**A mixed state is entangled if it cannot be written as mixture of factorizable pure states**

$$\hat{\rho} = \sum_k p_k \left(|\varphi_1^k\rangle \otimes |\varphi_2^k\rangle\right)\left(\langle\varphi_1^k| \otimes \langle\varphi_2^k|\right)$$

$$\hat{\rho} = \sum_k p_k\, \hat{\rho}_1^k \otimes \hat{\rho}_2^k$$




**check for separability - Schmidt decomposition**

$$|\Psi_{12}\rangle = \sum_{i=1}^{d_1} \sum_{j=1}^{d_2} c_{ij} |\phi_1^i\rangle \otimes |\phi_2^j\rangle \qquad r \leq \min\{d_1, d_2\}$$

$$|\Psi_{12}\rangle = \sum_{i=1}^{r} a_i |\psi_1^i\rangle \otimes |\psi_2^i\rangle \qquad a_i = \sqrt{p_i} > 0$$

# Bipartite quantum entanglement – pure states

The entropy of subsystem may be greater than the entropy of total system ($S_1 > S_{12}$) if and only if the system is entangled (classically forbidden).

**Entanglement of formation (Bennett, DiVincenzo) of a pure state $\varphi_{12}$** of bipartite quantum system is defined as von Neumann entropy of either member of the pair:

$$E(\varphi_{12}) = -\mathrm{Tr}\,\hat{\rho}_1 \log_2 \hat{\rho}_1 = -\mathrm{Tr}\,\hat{\rho}_2 \log_2 \hat{\rho}_2$$

$$\hat{\rho}_1 = \mathrm{Tr}_2\,\hat{\rho}_{12} = \mathrm{Tr}_2\,|\varphi_{12}\rangle\langle\varphi_{12}|$$
$$\hat{\rho}_2 = \mathrm{Tr}_1\,\hat{\rho}_{12} = \mathrm{Tr}_1\,|\varphi_{12}\rangle\langle\varphi_{12}|$$

**Schmidt decomposition:**

$$|\phi_{12}\rangle = \sum_{i=1}^{d_1}\sum_{j=1}^{d_2} c_{ij}|\tilde{\phi}_1^i\rangle|\tilde{\phi}_2^j\rangle \qquad r \le \min\{d_1, d_2\}$$

$$|\phi_{12}\rangle = \sum_{i=1}^{r} a_i|\phi_1^i\rangle|\phi_2^i\rangle \qquad a_i = \sqrt{p_i} > 0$$

$$\hat{\rho}_{12} = |\phi_{12}\rangle\langle\phi_{12}| = \sum_{i=1}^{r}\sum_{j=1}^{r} a_i a_j |\phi_1^i\rangle|\phi_2^i\rangle\langle\phi_1^j|\langle\phi_2^j|$$

$$\hat{\rho}_1 = \mathrm{Tr}_2\hat{\rho}_{12} = \mathrm{Tr}_2|\phi_{12}\rangle\langle\phi_{12}| = \sum_{k=1}^{r} a_k^2|\phi_1^k\rangle\langle\phi_1^k|$$

$$E(\varphi_{12}) = S(\hat{\rho}_1) = -\mathrm{Tr}\,\hat{\rho}_1 \log_2 \hat{\rho}_1 = -\sum_k a_k^2 \log_2 a_k^2 = -\sum_k p_k \log_2 p_k$$

# Bipartite quantum entanglement – mixed states

Entanglement of formation of a pure state $\varphi$ of a bipartite quantum system is then defined as von Neumann entropy of either member of the pair:

$$\hat{\rho}_1 = \mathrm{Tr}_2\, \hat{\rho}$$
$$\hat{\rho}_2 = \mathrm{Tr}_1\, \hat{\rho}$$

$$E(\varphi) = -\mathrm{Tr}\, \hat{\rho}_1 \log_2 \hat{\rho}_1 = -\mathrm{Tr}\, \hat{\rho}_2 \log_2 \hat{\rho}_2$$

Consider all possible pure-state decompositions of density matrix ρ of a pair of quantum systems numbered as 1 and 2, i.e. all ensembles of states $|\varphi_k\rangle$ with probabilities $p_k$ such that

$$\hat{\rho} = \sum_k p_k |\varphi_k\rangle\langle\varphi_k|$$

Entanglement of formation of a mixed state ρ of a bipartite quantum system is defined as the average entanglement of the pure states of the optimal decomposition minimized over all decompositions of ρ

$$E(\rho) = \min \sum_k p_k E(\varphi_k)$$

# Bipartite quantum entanglement - measures

A. Pure states: - spin-flip transformation for a single spin in a pure state:

$$|\tilde{\varphi}\rangle = \hat{\sigma}^y \, |\varphi\rangle^*$$

- spin-flip transformation for a spin pair in a pure state:

$$|\tilde{\varphi}\rangle = \hat{\sigma}^y \otimes \hat{\sigma}^y \, |\varphi\rangle^*$$

## Entanglement of formation

$$E(\psi) = \mathcal{E}(C(\psi)),$$

$$\mathcal{E}(C) = -\frac{1+\sqrt{1-C^2}}{2}\log_2\frac{1+\sqrt{1-C^2}}{2} - \frac{1-\sqrt{1-C^2}}{2}\log_2\frac{1-\sqrt{1-C^2}}{2}.$$

## Concurrence

$$C(\psi) = |\langle\psi|\tilde{\psi}\rangle|,$$

B. Mixed states: - spin-flip transformation for a spin pair in a mixed state:

$$\tilde{\rho} = (\,\hat{\sigma}^y \otimes \hat{\sigma}^y\,)\,\hat{\rho}^*(\,\hat{\sigma}^y \otimes \hat{\sigma}^y\,)$$

$$C = \max\{\sqrt{\lambda_1} - \sqrt{\lambda_2} - \sqrt{\lambda_3} - \sqrt{\lambda_4}, 0\}$$

$$R = \hat{\rho}(\hat{\sigma}^y \otimes \hat{\sigma}^y)\hat{\rho}^*(\hat{\sigma}^y \otimes \hat{\sigma}^y)$$

# Bipartite quantum entanglement - measures

A. Pure states: the most general pure state for a couple of spin-1/2 particles:

$$|\varphi\rangle = a|\uparrow\rangle_1|\uparrow\rangle_2 + b|\uparrow\rangle_1|\downarrow\rangle_2 + c|\downarrow\rangle_1|\uparrow\rangle_2 + d|\downarrow\rangle_1|\downarrow\rangle_2$$

**Concurrence:** $C = 2\,|bc - ad|$ $\quad 0 \le C \le 1$

$C = 0$: separable

$C = 1$: fully entangled

**Bell states ($C$=1):**

$$|\varphi_1\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle_1|\downarrow\rangle_2 - |\downarrow\rangle_1|\uparrow\rangle_2)$$

$$|\varphi_3\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle_1|\uparrow\rangle_2 - |\downarrow\rangle_1|\downarrow\rangle_2)$$

$$|\varphi_2\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle_1|\downarrow\rangle_2 + |\downarrow\rangle_1|\uparrow\rangle_2)$$

$$|\varphi_4\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle_1|\uparrow\rangle_2 + |\downarrow\rangle_1|\downarrow\rangle_2)$$

B. Mixed states: the most general mixed states for a couple of spin-1/2 particles:

$$\hat{\rho} = a|\uparrow\rangle_1|\uparrow\rangle_2\langle\uparrow|_1\langle\uparrow|_2 + b|\uparrow\rangle_1|\downarrow\rangle_2\langle\uparrow|_1\langle\downarrow|_2 + c|\downarrow\rangle_1|\uparrow\rangle_2\langle\downarrow|_1\langle\uparrow|_2 + d|\downarrow\rangle_1|\downarrow\rangle_2\langle\downarrow|_1\langle\downarrow|_2$$

$$\hat{\rho} = a|\varphi_1\rangle\langle\varphi_1| + b|\varphi_2\rangle\langle\varphi_2| + c|\varphi_3\rangle\langle\varphi_3| + d|\varphi_4\rangle\langle\varphi_4|$$

$$C = \max\{\sqrt{\lambda_1} - \sqrt{\lambda_2} - \sqrt{\lambda_3} - \sqrt{\lambda_4}, 0\}$$

$$R = \hat{\rho}(\hat{\sigma}^y \otimes \hat{\sigma}^y)\hat{\rho}^*(\hat{\sigma}^y \otimes \hat{\sigma}^y)$$

# Quantum statistical mechanics – canonical ensemble

**density operator**

$$\hat{\rho} = \frac{1}{Z}\exp(-\beta\hat{\mathcal{H}}) = \frac{\exp(-\beta\hat{\mathcal{H}})}{\mathrm{Tr}\exp(-\beta\hat{\mathcal{H}})}$$

$$\beta = 1/(k_{\mathrm{B}}T)$$

**statistical mean values**

$$\langle\hat{A}\rangle = \mathrm{Tr}(\hat{\rho}\hat{A})$$

**concurrence**

$$C = \max\{\sqrt{\lambda_1} - \sqrt{\lambda_2} - \sqrt{\lambda_3} - \sqrt{\lambda_4}, 0\}$$

$$R = \hat{\rho}(\hat{\sigma}^y \otimes \hat{\sigma}^y)\hat{\rho}^*(\hat{\sigma}^y \otimes \hat{\sigma}^y)$$

**entanglement of formation**

$$\mathcal{E}(C) = -\frac{1+\sqrt{1-C^2}}{2}\log_2\frac{1+\sqrt{1-C^2}}{2} - \frac{1-\sqrt{1-C^2}}{2}\log_2\frac{1-\sqrt{1-C^2}}{2}.$$

# Spin-1/2 Heisenberg dimer:



$$\hat{\rho} = \frac{1}{Z}\exp(-\beta\hat{\mathcal{H}}) = \frac{\exp(-\beta\hat{\mathcal{H}})}{\mathrm{Tr}\exp(-\beta\hat{\mathcal{H}})} \qquad \beta = 1/(k_{\mathrm{B}}T)$$

## - Hamiltonian and its matrix form

$$\hat{\mathcal{H}} = J\hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_2 - h(\hat{S}_1^z + \hat{S}_2^z)$$

$$\langle\gamma|\hat{\mathcal{H}}|\alpha\rangle = \begin{pmatrix} \langle\uparrow\uparrow|\hat{\mathcal{H}}|\uparrow\uparrow\rangle & \langle\uparrow\downarrow|\hat{\mathcal{H}}|\uparrow\uparrow\rangle & \langle\downarrow\uparrow|\hat{\mathcal{H}}|\uparrow\uparrow\rangle & \langle\downarrow\downarrow|\hat{\mathcal{H}}|\uparrow\uparrow\rangle \\ \langle\uparrow\uparrow|\hat{\mathcal{H}}|\uparrow\downarrow\rangle & \langle\uparrow\downarrow|\hat{\mathcal{H}}|\uparrow\downarrow\rangle & \langle\downarrow\uparrow|\hat{\mathcal{H}}|\uparrow\downarrow\rangle & \langle\downarrow\downarrow|\hat{\mathcal{H}}|\uparrow\downarrow\rangle \\ \langle\uparrow\uparrow|\hat{\mathcal{H}}|\downarrow\uparrow\rangle & \langle\uparrow\downarrow|\hat{\mathcal{H}}|\downarrow\uparrow\rangle & \langle\downarrow\uparrow|\hat{\mathcal{H}}|\downarrow\uparrow\rangle & \langle\downarrow\downarrow|\hat{\mathcal{H}}|\downarrow\uparrow\rangle \\ \langle\uparrow\uparrow|\hat{\mathcal{H}}|\downarrow\downarrow\rangle & \langle\uparrow\downarrow|\hat{\mathcal{H}}|\downarrow\downarrow\rangle & \langle\downarrow\uparrow|\hat{\mathcal{H}}|\downarrow\downarrow\rangle & \langle\downarrow\downarrow|\hat{\mathcal{H}}|\downarrow\downarrow\rangle \end{pmatrix} = \begin{pmatrix} \frac{J}{4}-h & 0 & 0 & 0 \\ 0 & -\frac{J}{4} & \frac{J}{2} & 0 \\ 0 & \frac{J}{2} & -\frac{J}{4} & 0 \\ 0 & 0 & 0 & \frac{J}{4}+h \end{pmatrix}$$

## - Pauli spin operators and basis

$$\hat{S}_j^x = \frac{1}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}_j, \quad \hat{S}_j^y = \frac{1}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}_j, \quad \hat{S}_j^x = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}_j,$$

$$|\uparrow\uparrow\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}_1 \begin{pmatrix} 1 \\ 0 \end{pmatrix}_2, \quad |\uparrow\downarrow\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}_1 \begin{pmatrix} 0 \\ 1 \end{pmatrix}_2,$$

$$|\downarrow\uparrow\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}_1 \begin{pmatrix} 1 \\ 0 \end{pmatrix}_2, \quad |\downarrow\downarrow\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}_1 \begin{pmatrix} 0 \\ 1 \end{pmatrix}_2.$$

## - concurrence (Wootters, 1998):

$$C = \max\{\sqrt{\lambda_1} - \sqrt{\lambda_2} - \sqrt{\lambda_3} - \sqrt{\lambda_4}, 0\}$$

$$R = \hat{\rho}(\hat{\sigma}^y \otimes \hat{\sigma}^y)\hat{\rho}^*(\hat{\sigma}^y \otimes \hat{\sigma}^y)$$

# Spin-1/2 Heisenberg dimer:

## - Hamiltonian and its matrix form:

$$\hat{\mathcal{H}} = J\hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_2 - h(\hat{S}_1^z + \hat{S}_2^z) = \begin{pmatrix} \frac{J}{4} - h & 0 & 0 & 0 \\ 0 & -\frac{J}{4} & \frac{J}{2} & 0 \\ 0 & \frac{J}{2} & -\frac{J}{4} & 0 \\ 0 & 0 & 0 & \frac{J}{4} + h \end{pmatrix}$$

$$\beta = 1/(k_{\mathrm{B}}T)$$

## - Energy spectrum and eigenvectors:

$$E_0 = -\frac{3}{4}J \qquad |\phi_0\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$$

$$E_1 = \frac{1}{4}J - h \qquad |\phi_1\rangle = |\uparrow\uparrow\rangle$$

$$E_2 = \frac{1}{4}J \qquad |\phi_2\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)$$

$$E_3 = \frac{1}{4}J + h \qquad |\phi_3\rangle = |\downarrow\downarrow\rangle$$

## - Spectral decomposition:

$$\hat{\rho} = \frac{1}{Z}\exp(-\beta\hat{\mathcal{H}}) = \frac{\exp(-\beta\hat{\mathcal{H}})}{\mathrm{Tr}\exp(-\beta\hat{\mathcal{H}})}$$

$$\hat{\rho} = \frac{\sum_{i=0}^{3} \exp(-\beta E_i)\ |\varphi_i\rangle\langle\varphi_i|}{\sum_{i=0}^{3} \exp(-\beta E_i)}$$

## - concurrence (Wootters, 1998):

$$C = \max\{\sqrt{\lambda_1} - \sqrt{\lambda_2} - \sqrt{\lambda_3} - \sqrt{\lambda_4}, 0\}$$

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- **concurrence (Wootters, 1998):**

$$C = \max\{\sqrt{\lambda_1} - \sqrt{\lambda_2} - \sqrt{\lambda_3} - \sqrt{\lambda_4}, 0\}$$

$$R = \hat{\rho}(\hat{\sigma}^y \otimes \hat{\sigma}^y)\hat{\rho}^*(\hat{\sigma}^y \otimes \hat{\sigma}^y)$$

- **density matrix and eigenvalues of *R*:**

$$\hat{\rho} = \frac{1}{2[1+\mathrm{e}^{\beta J} + 2\cosh(\beta h)]} \times \begin{pmatrix} 2\mathrm{e}^{\beta h} & 0 & 0 & 0 \\ 0 & 1+\mathrm{e}^{\beta J} & 1-\mathrm{e}^{\beta J} & 0 \\ 0 & 1-\mathrm{e}^{\beta J} & 1+\mathrm{e}^{\beta J} & 0 \\ 0 & 0 & 0 & 2\mathrm{e}^{-\beta h} \end{pmatrix}$$

$$\lambda_1 = \left[\frac{\mathrm{e}^{\beta J}}{1+\mathrm{e}^{\beta J} + 2\cosh(\beta h)}\right]^2$$

$$\lambda_2 = \lambda_3 = \lambda_4 = \left[\frac{1}{1+\mathrm{e}^{\beta J} + 2\cosh(\beta h)}\right]^2$$

- **Concurrence and threshold (sudden-death) temperature:**

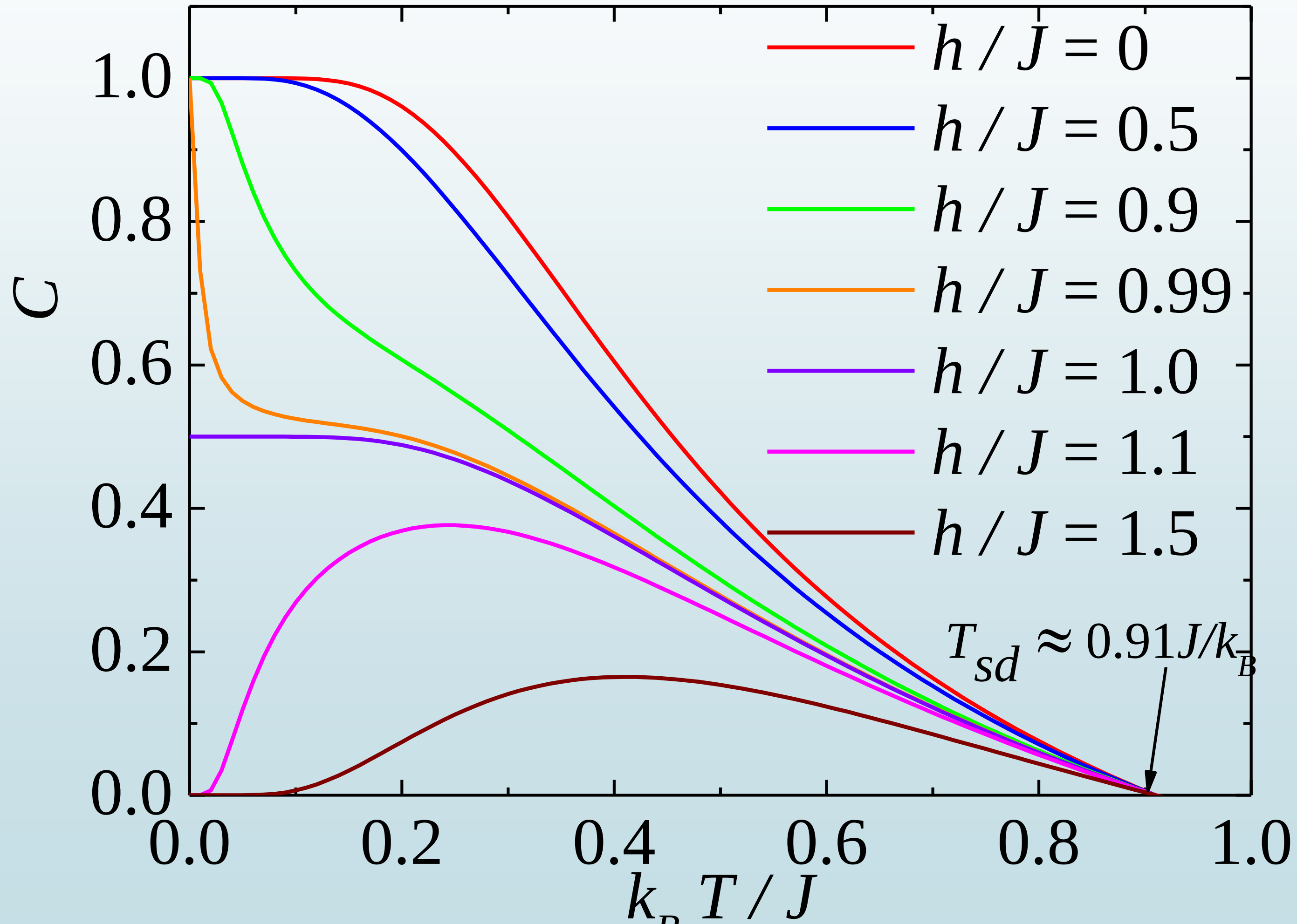
$$C = \max\left(\frac{\exp(\beta J) - 3}{\exp(\beta J) + 1 + 2\cosh(\beta h)}, 0\right) \qquad T_{sd} = \frac{J}{k_B \ln 3}$$

## Spin-1/2 Heisenberg antiferromagnetic dimer:

### - concurrence and threshold (sudden-death) temperature:

$$C = \max\left(\frac{\exp(\beta J)-3}{\exp(\beta J)+1+2\cosh(\beta h)}, 0\right)$$

$$T_{sd} = \frac{J}{k_B \ln 3}$$




A full entanglement at zero temperature due to singlet ground state

$$|S\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\rangle_1|\downarrow\rangle_2 - |\downarrow\rangle_1|\uparrow\rangle_2\right)$$

Entanglement is suppressed by a magnetic field, but a threshold temperature does not depend on a magnetic field!

# Spin-1/2 Heisenberg dimer:

$$\hat{\rho} = \frac{1}{Z}\exp(-\beta\hat{\mathcal{H}}) = \frac{\exp(-\beta\hat{\mathcal{H}})}{\mathrm{Tr}\exp(-\beta\hat{\mathcal{H}})} \qquad \beta = 1/(k_{\mathrm{B}}T)$$

- concurrence (Wooters, 1998):

$$C = \max\{\sqrt{\lambda_1} - \sqrt{\lambda_2} - \sqrt{\lambda_3} - \sqrt{\lambda_4}, 0\}$$

$$R = \hat{\rho}(\hat{\sigma}^y \otimes \hat{\sigma}^y)\hat{\rho}^*(\hat{\sigma}^y \otimes \hat{\sigma}^y)$$

- density matrix in a matrix representation:

$$\hat{\rho} = \begin{pmatrix} u_+ & 0 & 0 & 0 \\ 0 & v_+ & z & 0 \\ 0 & z & v_- & 0 \\ 0 & 0 & 0 & u_- \end{pmatrix},$$

$$u_\pm = \tfrac{1}{4} \pm M_z + q_{zz}$$
$$v_\pm = \tfrac{1}{4} \pm \delta S_z - q_{zz}$$
$$z = 2q_{xx},$$

$$\begin{aligned} M_z &= \frac{1}{2}\langle \hat{S}_1^z + \hat{S}_1^z \rangle \\ \delta S_z &= \frac{1}{2}\langle \hat{S}_1^z - \hat{S}_1^z \rangle \\ q_{zz} &= \langle \hat{S}_1^z \hat{S}_1^z \rangle \\ q_{xx} &= \langle \hat{S}_1^x \hat{S}_1^x \rangle \end{aligned}$$

- concurrence in terms of local observables (Amico, 2004):

$$\mathcal{C} = 2\max\left\{0, 2|q_{xx}| - \sqrt{\left(\frac{1}{4} + q_{zz}\right)^2 - M_z^2}\right\}.$$

# Spin-1/2 Heisenberg dimer: experimental perspective

EPL, **113** (2016) 40004
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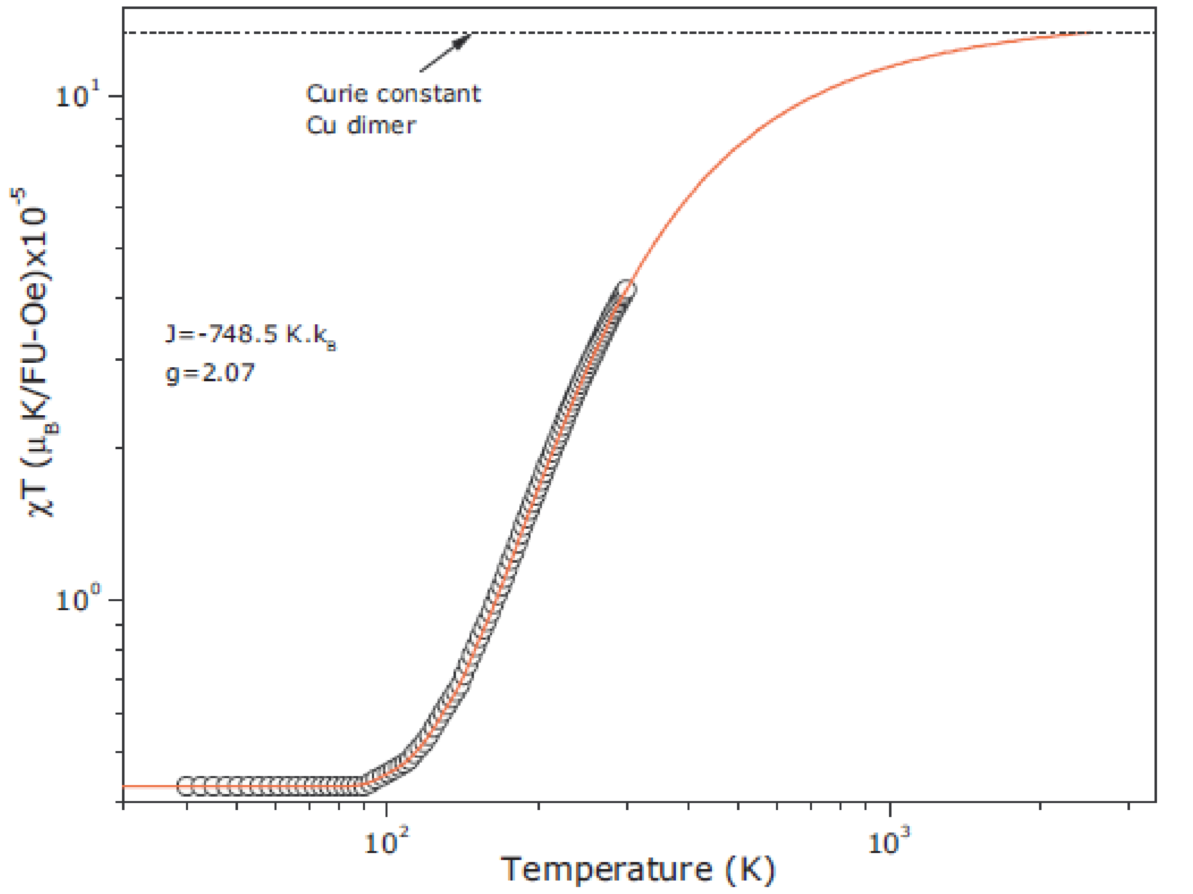
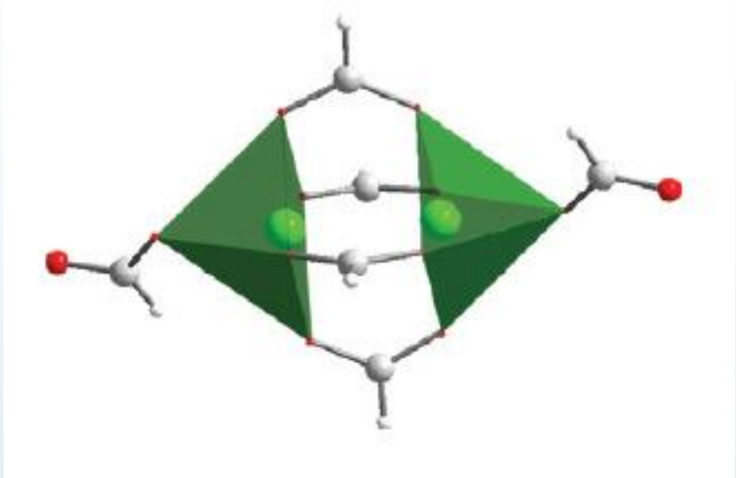
www.epljournal.org

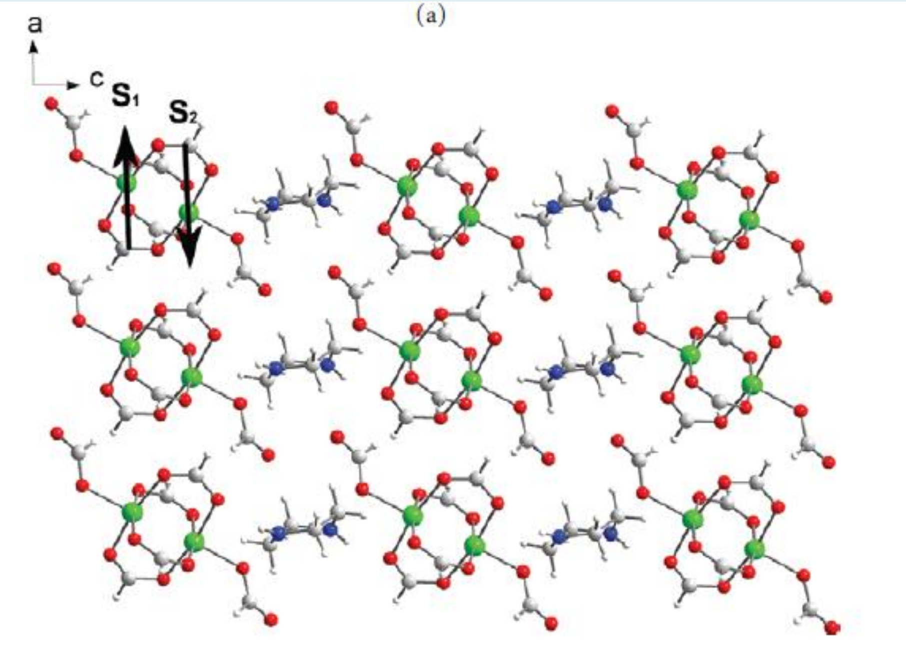
## Carboxylate-based molecular magnet: One path toward achieving stable quantum correlations at room temperature

C. Cruz[1(a)], D. O. Soares-Pinto[2], P. Brandão[3], A. M. dos Santos[4] and M. S. Reis[1]

[Cu2(HCOO)4(HCOOH)2(piperazine)]





# Spin-1/2 Heisenberg dimer: theory vs. experiment

- zero-field susceptibility:

$$\chi(T) = \frac{2N(g\mu_B)^2}{k_B T}\frac{1}{3+e^{-J/k_B T}}$$

- fluctuation-dissipation theorem:

$$q(T) = \frac{k_B T}{2N(g\mu_B)^2}\chi(T) - \frac{1}{4}$$

- concurrence (general):

$$\mathcal{C} = 2\max\left\{0, 2|q_{xx}| - \sqrt{\left(\frac{1}{4}+q_{zz}\right)^2 - M_z^2}\right\}.$$

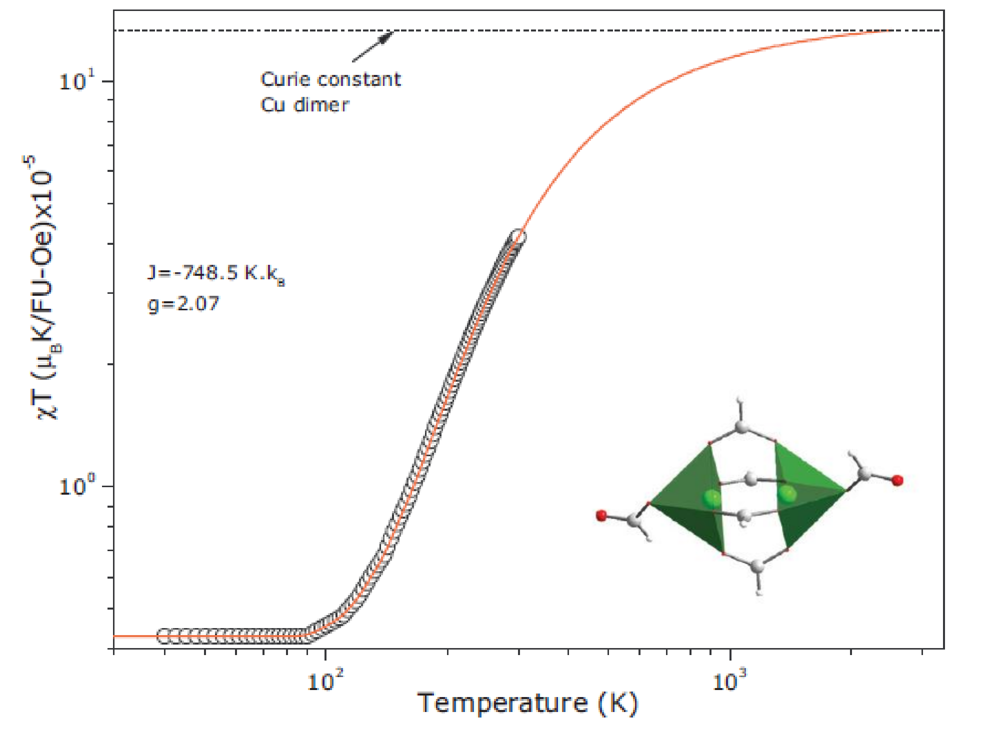
- concurrence (zero field):

$$C = 2\max\left\{3|q| - \frac{1}{4}, 0\right\} \qquad q_{xx} = q_{zz} \equiv q$$

- entanglement of formation:

$$E_F(\rho) = -\sum_{\sigma=\pm}\frac{\sqrt{1+\sigma C^2(\rho)}}{2}\ln\frac{\sqrt{1+\sigma C^2(\rho)}}{2},$$

[Cu2(HCOO)4(HCOOH)2(piperazine)]



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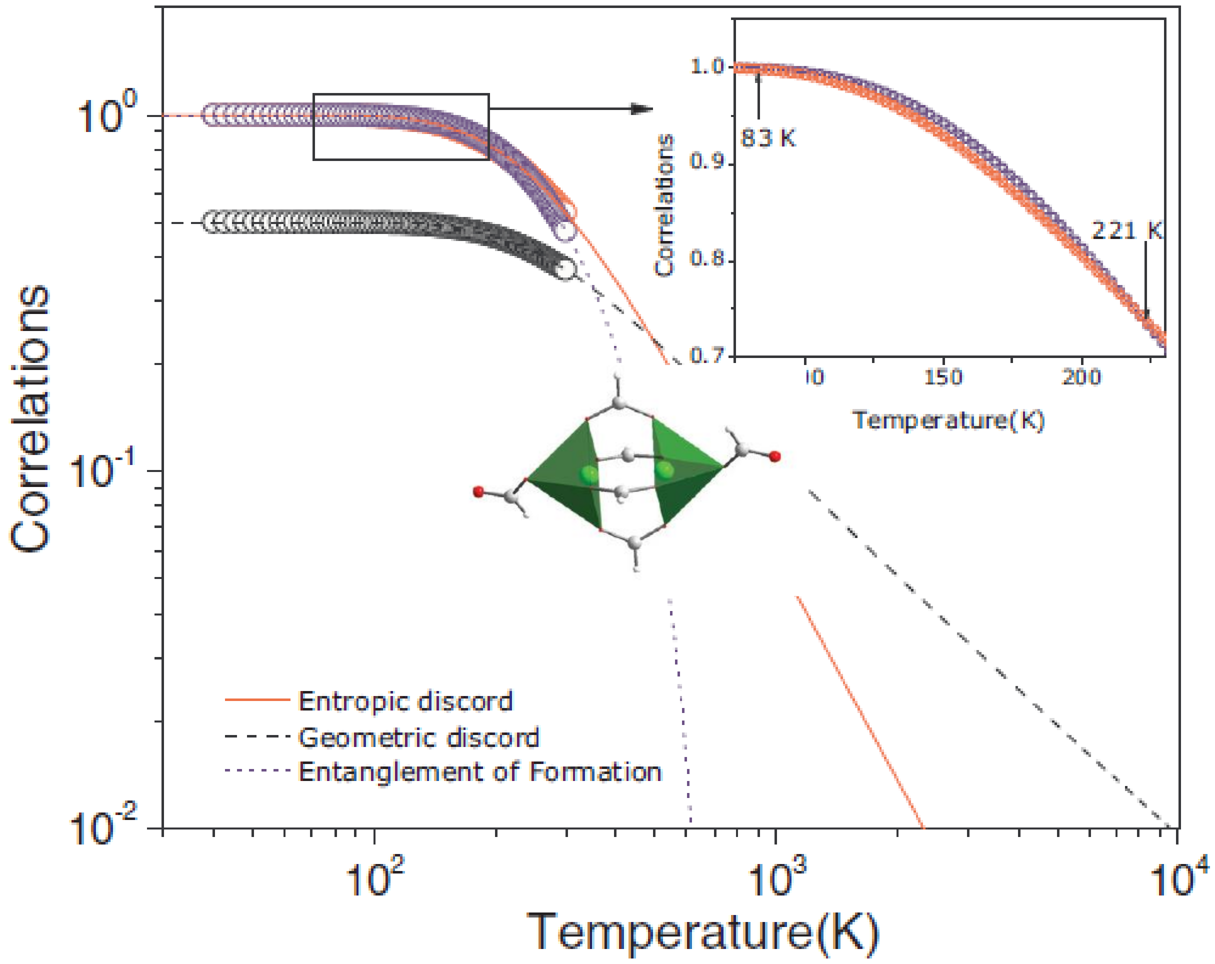
$$E_F(\rho) = -\sum_{\sigma=\pm}\frac{\sqrt{1+\sigma C^2(\rho)}}{2}\ln\frac{\sqrt{1+\sigma C^2(\rho)}}{2},$$

[Cu2(HCOO)4(HCOOH)2(piperazine)]



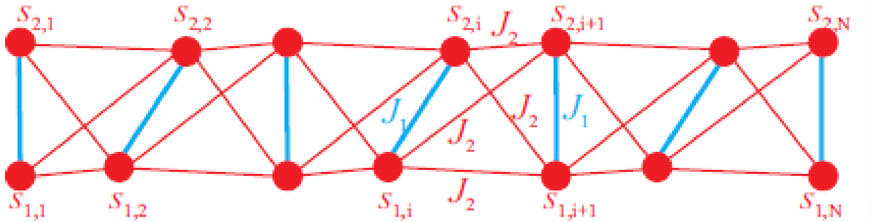

- sudden-death temperature

$$\frac{k_B T_{sd}}{|J|} = \frac{1}{\ln 3} \approx 0.910239\ldots$$

# Magnetization process, bipartite entanglement, and enhanced magnetocaloric effect of the exactly solved spin-1/2 Ising-Heisenberg tetrahedral chain

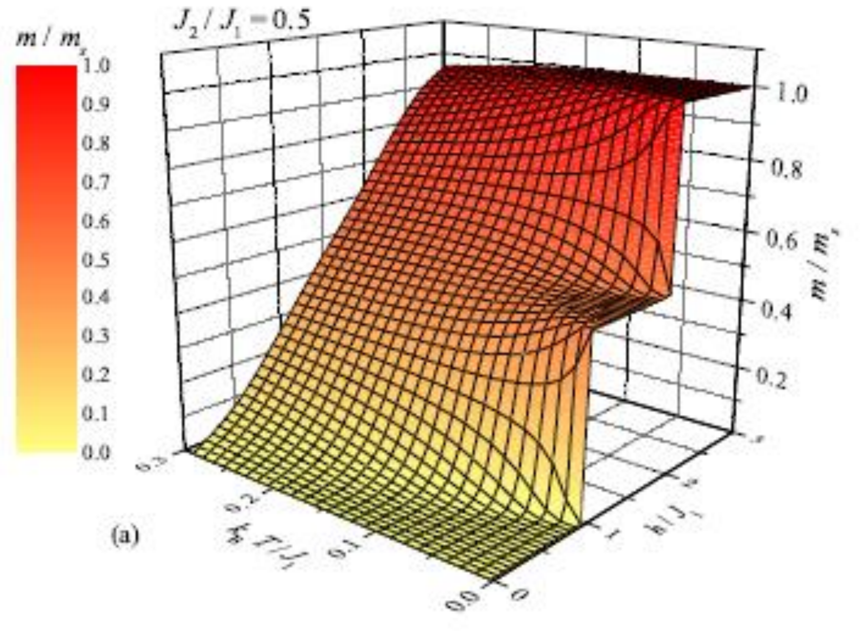
Jozef Strečka,[1,*] Onofre Rojas,[2] Taras Verkholyak,[3] and Marcelo L. Lyra[4]

PHYSICAL REVIEW E 89, 022143 (2014)

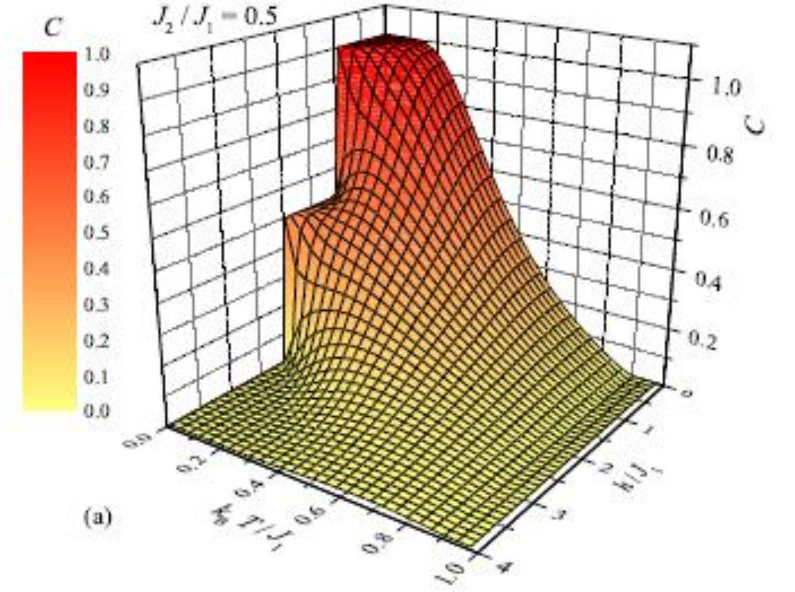



## Magnetization and Concurrence

SD→SB→FM




SD→SB→FM

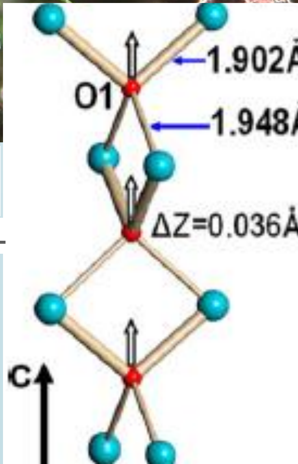



## K4Cu4O2(SO4).4MeCl

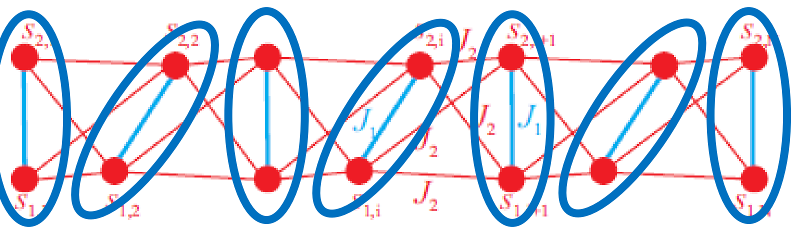
L. M. Volkova[1] · D. V. Marinin[1]

J Supercond Nov Magn (2017) 30:959-

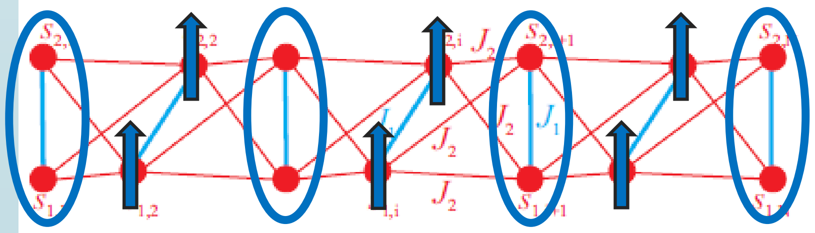
## Piypite




## Singlet-dimer (SD)



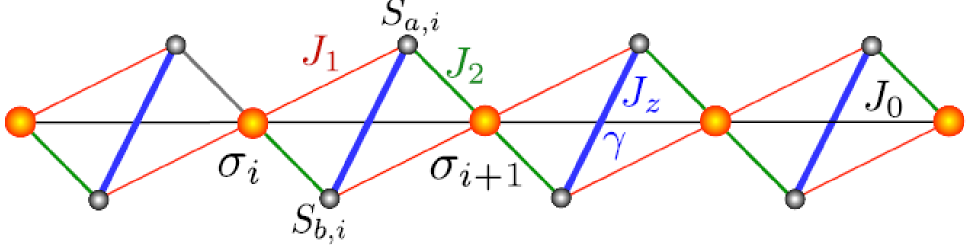
## Staggered bond (SB)



# Thermal entanglement in a spin-1/2 Ising-XYZ distorted diamond chain with the second-neighbor interaction between nodal Ising spins

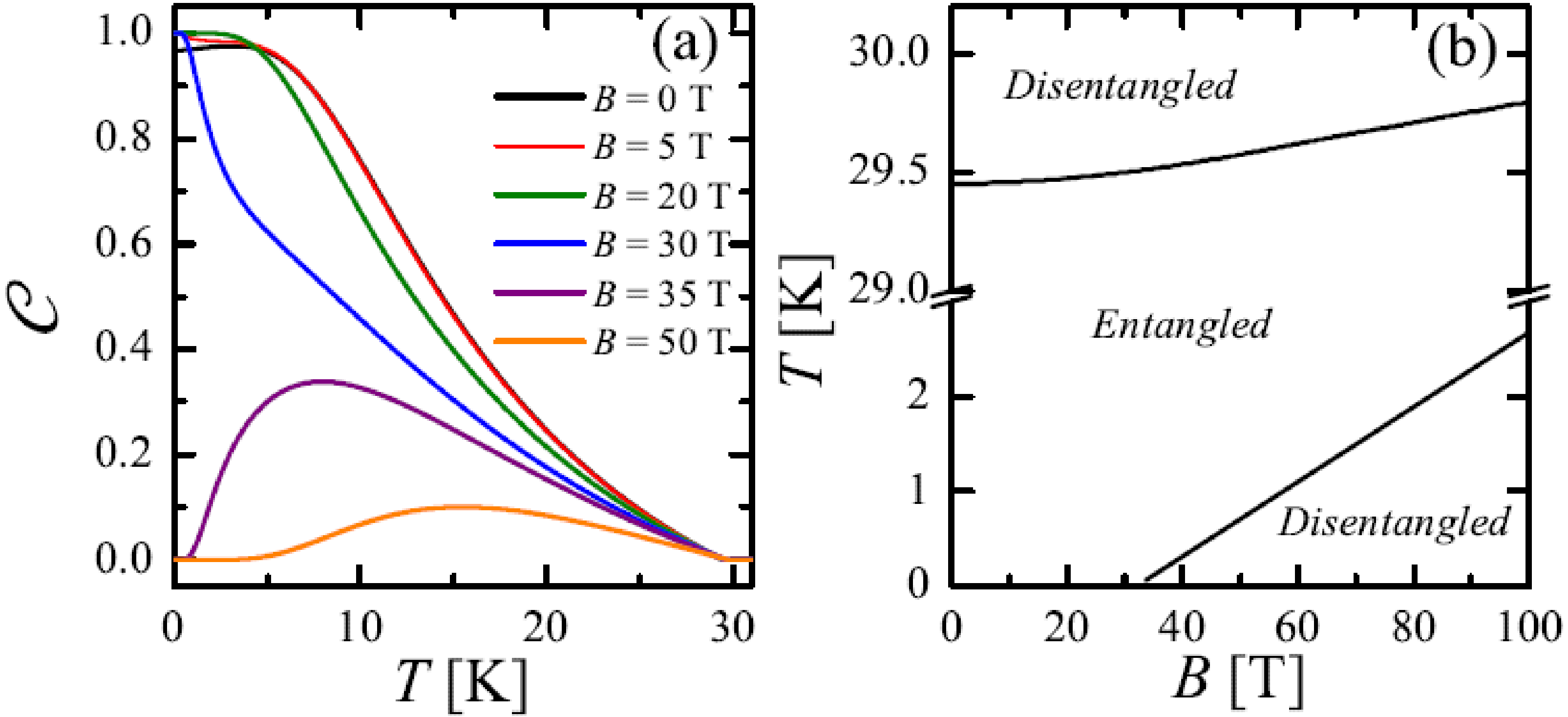
Physica A 486 (2017) 367–377

Onofre Rojas [a], M. Rojas [a], S.M. de Souza [a], J. Torrico [b,*], J. Strečka [c], M.L. Lyra [b]




$Cu_3(CO_3)_2(OH)_2$

## Bipartite entanglement in azurite





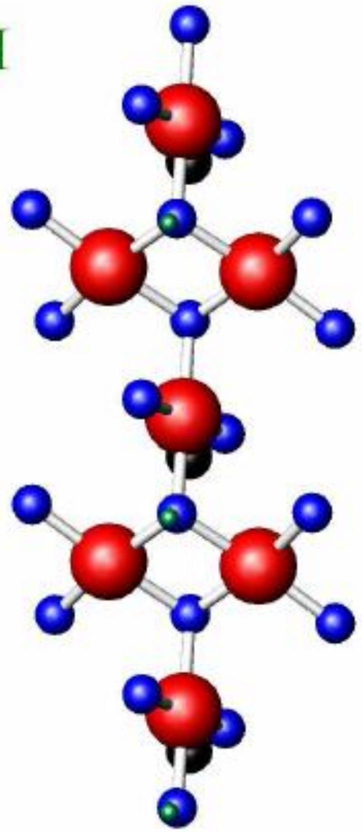
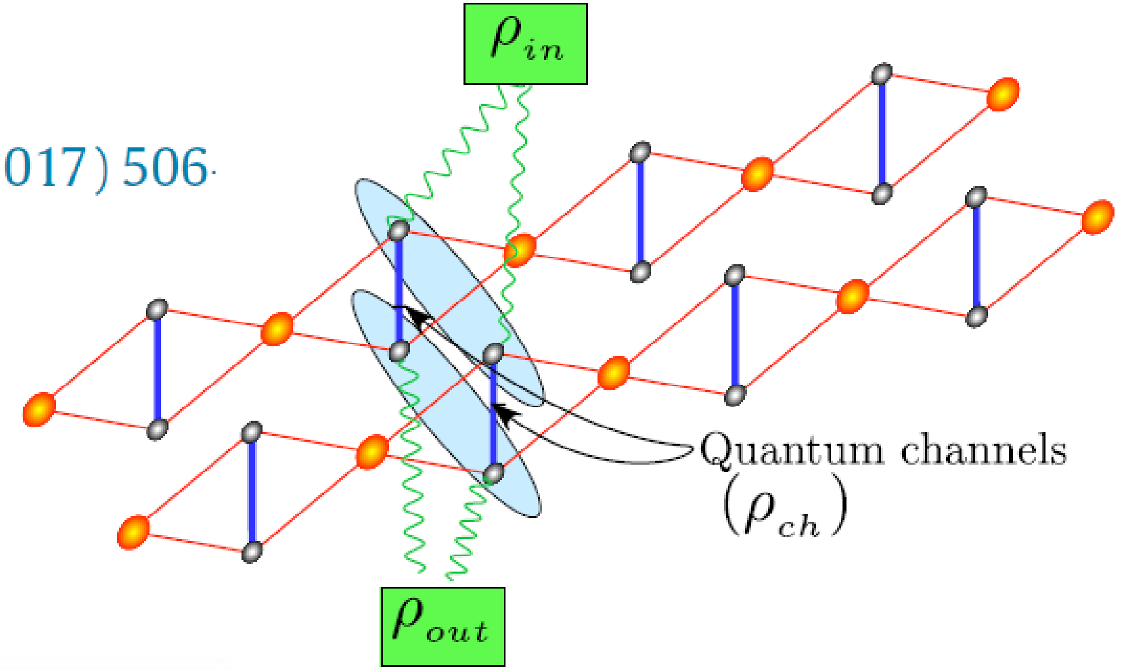



Fig. 7. (Color online) (a) The temperature dependence of the concurrence for several values of the magnetic field $B$ and the coupling constants $J/k_B = J_z/k_B = 33$ K, $J_1/k_B = 15.5$ K, $J_2/k_B = 6.9$ K, $J_0/k_B = 4.6$ K, $\gamma = 0$, $g = 2.06$ relevant to the azurite; (b) the threshold temperature as a function of magnetic field $B$ for the coupling constants relevant to the azurite.

# Entangled state teleportation through a couple of quantum channels composed of *XXZ* dimers in an Ising-*XXZ* diamond chain

Annals of Physics 377 (2017) 506

M. Rojas [a,*], S.M. de Souza [a], Onofre Rojas [a,b]

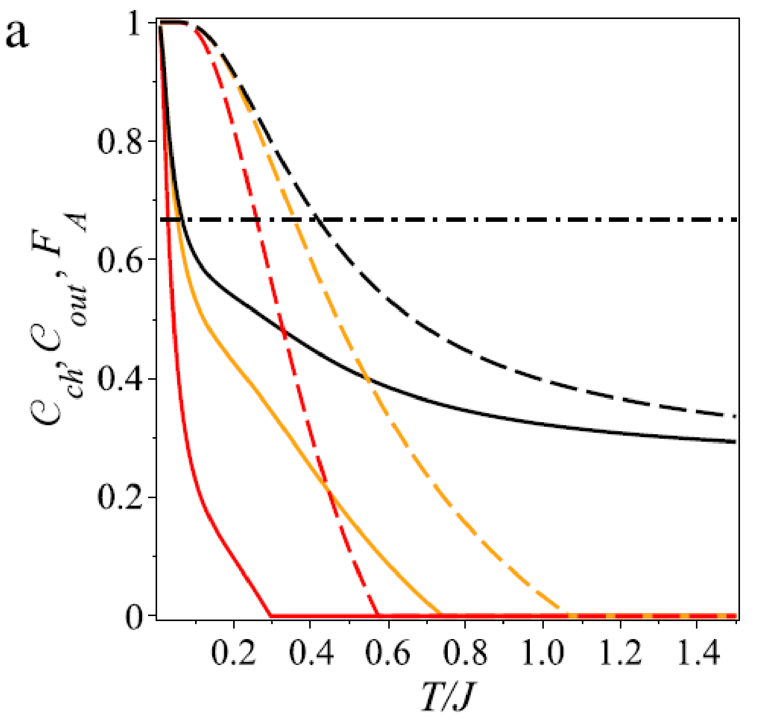


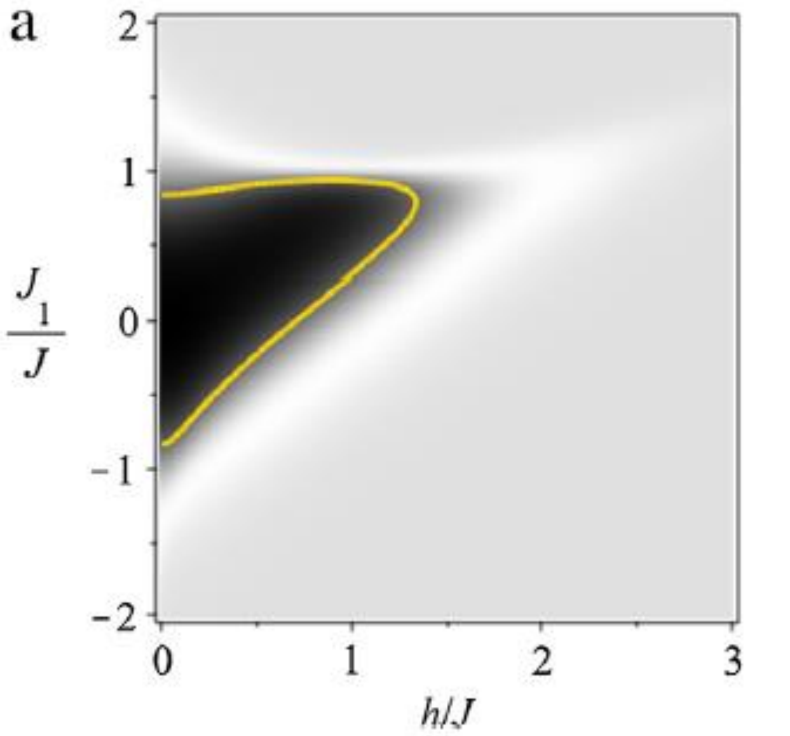

**Output**

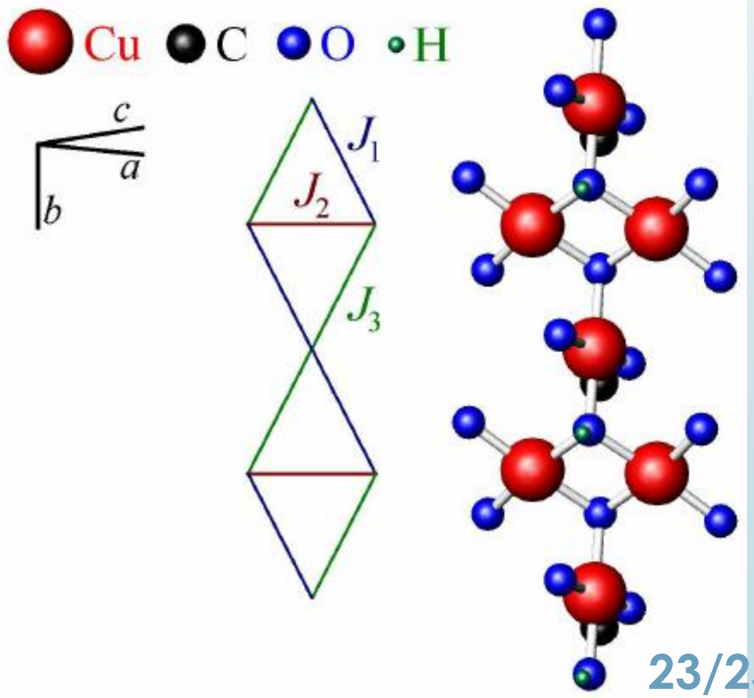
$$\rho_{out} = \sum_{i,j=\{0,x,y,z\}} p_i p_j (\sigma_i \otimes \sigma_j) \rho_{in} (\sigma_i \otimes \sigma_j),$$

**Fidelity**

$$F = \left\{ \mathrm{tr}\left[ \sqrt{\sqrt{\rho_{in}}\rho_{out}\sqrt{\rho_{in}}} \right] \right\}^2$$



# Other measures of bipartite entanglement

$$\hat{\rho} = \frac{1}{Z}\exp(-\beta\hat{\mathcal{H}}) = \frac{\exp(-\beta\hat{\mathcal{H}})}{\mathrm{Tr}\exp(-\beta\hat{\mathcal{H}})}$$

$$\beta = 1/(k_{\mathrm{B}}T)$$

- concurrence (Wootters, 1998):

$$C = \max\{\sqrt{\lambda_1} - \sqrt{\lambda_2} - \sqrt{\lambda_3} - \sqrt{\lambda_4}, 0\}$$

$$R = \hat{\rho}(\hat{\sigma}^y \otimes \hat{\sigma}^y)\hat{\rho}^*(\hat{\sigma}^y \otimes \hat{\sigma}^y)$$

- entanglement of formation (Wootters, 1998):

$$\mathcal{E}(C) = -\frac{1+\sqrt{1-C^2}}{2}\log_2\frac{1+\sqrt{1-C^2}}{2} - \frac{1-\sqrt{1-C^2}}{2}\log_2\frac{1-\sqrt{1-C^2}}{2}.$$

- negativity (Peres, 1996):

$$\mathcal{N} = \sum_{\lambda<0}\lambda,$$

$$\langle m|\langle\mu|\varrho_{AB}^{T_B}|n\rangle|\nu\rangle \equiv \langle m|\langle\nu|\varrho_{AB}|n\rangle|\mu\rangle$$

- von Neumann entropy (Schumacher, 1995):

$$S(A|B) = S(\rho_{AB}) - S(\rho_B),$$

$$S(\hat{\rho}) = -\mathrm{Tr}\,\hat{\rho}\log_2\hat{\rho}$$

- fidelity (Richard, 1994):

$$F = \mathrm{Tr}\sqrt{\hat{\rho}(T)\hat{\rho}(T+\delta T)}$$

-Clauser-Horne-Shimony-Holt (Bell-type) inequality (Horodecki, 1995)

$$\mathcal{B}(\hat{\rho}) = 2\sqrt{\lambda_1+\lambda_2} \leq 2.$$

$$\mathcal{L}_{ij}(\hat{\rho}) = \mathrm{Tr}[\hat{\rho}\cdot\hat{\sigma}_i \otimes \hat{\sigma}_j],$$

# Quantum entanglement between spins in magnetic systems

- theoretically accessible via density matrix

- bipartite entanglement persists up to temperatures proportional to the exchange coupling J/k

- effect of temperature and magnetic field

- experimentally accessible through measurements

  1. *zero field: susceptibility, specific heat*
  2. *non-zero field: plus magnetization*
  3. *local probes (INS, NMR)*

## Open and challenging problems:

- *Beyond small spin clusters and chains ???*
- *itinerant magnetism - fermionic entanglement ???*
- *multipartite entanglement ???*
- *technological applications ???*