Quantifying quantum coherence in a metal-silicate framework

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Abstract – In this work we report an application of coherence theory to a low-dimensional molecular magnetic system, through the study of temperature, pressure and magnetic fields influence on the quantum coherence of a Cu(II) metal-silicate framework as a function of the magnetic susceptibility of the compound. Our results show that the quantum coherence of a low-dimensional molecular magnetic system can be handled by the management of the external conditions, offering an alternative way to identify quantum coherence through magnetometric experiments.

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Introduction. – The development of new technologies has provided great advances in materials preparation techniques, leading to the emergence of new electronic devices. Nowadays, we have reached the point where the miniaturization of these devices has led to the development of molecular-size components. However, designing molecular components requires a deep understanding of the quantum properties of these components. The technological challenges of quantum information science led us to consider fundamental aspects of molecular magnetism, because of its ease of synthesis, great versatility, and low-dimensional quantum features [1–12].

In recent years, it has been demonstrated that molecular magnetic systems present themselves as strong candidates as prototype materials for emerging quantum devices, and the characterization of their quantum correlations has received a considerable attention [2,4–8,12–15]. Recently, it has been demonstrated that these systems may be immune to decoherence mechanisms, presenting highly stable quantum correlations against external perturbations such as temperature and magnetic fields [2,4–8,12–15]. On the other hand, while the entanglement and non-classical correlations (or quantum correlations) are a key resource to characterize the quantum properties of a bipartite and some multipartite systems, quantum coherence is a common necessary condition for different forms of quantum correlations [16–20], being a fundamental feature for signifying quantumness in an integral system [17].

Quantum coherence, arising from the coherent superposition of quantum states, is a remarkable feature in quantum optics, quantum information theory, solid state physics, quantum game theory, quantum metrology and thermodynamics [16–33]. Recently a criterion of measurement that quantifies quantum coherence in solid states was proposed by Baumgratz et al. [34]. The authors established the fundamental assumptions for a quantitative theory of coherence, enabling the development of a rigorous theory of quantum coherence as a physical resource [27]. However, in order to utilize the remarkable features of quantum coherence it is necessary to define a consistent theoretical basis to measure it experimentally.

In the present work, we report a study of the $l_1$ trace norm quantum coherence [17,27,34,35] in an antiferromagnetic metal-silicate framework, formed in the compound KNaCuSi$_4$O$_{10}$ [12,36]. We establish a relationship between the measurement of quantum coherence and the magnetic susceptibility of the compound, which allows us to estimate the degree quantum coherence directly from a set of experimental data. We characterize the degree of quantum coherence in this molecular magnetic system in thermal equilibrium and investigate the influence of the temperature, pressure and magnetic fields. Our results
show that, similarly to entanglement and quantum discord [2,4–8,12–15], it is possible to handle the degree of coherence in a low-dimensional molecular magnetic system by controlling those external conditions, offering an alternative way to describe the quantum coherence in a condensed matter system through a thermodynamic property, opening a large avenue for research towards the development of novel materials with enhanced quantum properties employing materials engineering.

Quantum coherence in a molecular magnetic system. — Geometric approaches are widely used to characterize and quantify the quantum correlations in a wide variety of quantum systems. Similarly to the approach proposed in the entanglement theory [37], from which the entanglement can be characterized by a distance between the considered state and a set of states closed under LOCC operations (separable states) [17,34,37–39], Baumgratz et al. [34] provide one path towards quantifying the amount of coherence in a quantum state. From this consideration, Baumgratz et al. [34] showed that the operator that describes the quantum state of the system under investigation or by a task for which coherence is defined by the physical nature of the problem may be measured by the trace norm quantum coherence to characterize and quantify the quantum correlations in a wide variety of quantum states. Note that the Bleany-Bowers equation, eq. (4), where the authors obtained $J/k_B = -2.86(3)$ K (antiferromagnetic coupled ions).

To go further and analyze the quantum coherence by means of the magnetic susceptibility of the material in thermal equilibrium, firstly, we write the density matrix of the system under consideration in the local $S_z$ eigenbasis $\{|00\rangle, |01\rangle, |10\rangle, |11\rangle\}$, [12,43,44]:

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

where $g$ is the Landé factor, $\mu_B$ is the Bohr magneton, $k_B$ is the Boltzmann constant and $N$ is the number of dimers. Magnetic susceptibility measurements for the KNaCuSi$_4$O$_{10}$ compound are presented in ref. [36], where the measurements have been performed between 2 K and 350 K. Taking into account the crystal structure of this compound, the susceptibility data have been fitted to the Bleany-Bowers equation, eq. (4), where the authors obtain $J/k_B = -2.86(3)$ K (antiferromagnetic coupled ions).

To further analyze the quantum coherence by means of the magnetic susceptibility of the material in thermal equilibrium, firstly, we write the density matrix of the system under consideration in the local $S_z$ eigenbasis $\{|00\rangle, |01\rangle, |10\rangle, |11\rangle\}$, [12,43,44]:

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In order to study the role of external parameters, such as temperature, pressure and magnetic fields, on the quantum coherence of a molecular magnetic system, we will take the reference basis as one of the spin eigenbasis in a certain direction within a quantum metrology setting. For the temperature dependence on the quantum coherence, from an experimental point of view, we associate the calculation of the trace norm quantum coherence to the measurement of magnetic susceptibility.

Experimental determination of thermal quantum coherence. — The material, in which we evaluate the quantum coherence, is the KNaCuSi$_4$O$_{10}$ compound [12,36,40], a metal-silicate framework formed by Cu(II) spin dimers. This material was chosen because it has synthetic analogs of the naturally occurring mineral litidionite [36], being an ideal realization of a two-qubit system [12], since these dimers are magnetically isolated from each other, separated by two SiO$_4$ corners [36].

Therefore, this prototype material can be described by a two-qubit system interacting by the Heisenberg model [1,12,36,41],

$$\mathcal{H} = -J\vec{S}_1 \cdot \vec{S}_2,$$

where $J$ is the coupling constant. The magnetic susceptibility of this prototype material corresponds to the Bleany-Bowers equation [1,42]:

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by measuring the thermodynamic properties of solids, such as magnetic susceptibility.

In fig. 1, we show the quantum coherence obtained from the measurement of the magnetic susceptibility of our prototype material KNaCuSi$_4$O$_{10}$, reported in ref. [36]. The theoretical curves were plotted taking the corresponding estimates for the coupling constant $J/k_B$ in eq. (7). Reference [4] investigates the thermal quantum entanglement of this prototype material finding the maximum temperature of 2.43(7) K below which there is quantum entanglement between the Cu(II) ions; at this temperature the coherence of the system is 35% of the maximum value. As can be seen, as expected, increasing the temperature changes the Boltzmann weights due to the thermal fluctuations, which changes the occupation of the energy levels, leading the system to populate incoherent states.

On the other hand, apart from its quantification and characterization, the coherence is intimately associated with other quantum correlations quantifiers [45,46]. Thus, quantum coherence and correlations can be transformed into each other. The quantum discord [47], a measurement of quantum correlations beyond entanglement [2,27,46], can also be quantified in a molecular magnetic system via a distance-based approach [2,3,12]. In this regard, eq. (7) relates to the geometric quantum discord based on the Schatten 1-norm [48] as

$$Q_G(\rho) = \min_{\omega_{cq}} \| \rho - \rho_c \| = \frac{C(T)}{2},$$

where $\| A \|_1 = \text{Tr} \left[ \sqrt{A^\dagger A} \right]$, $\rho$ is a given quantum state and $\rho_c$ is the closest classical-quantum state [49,50]. Therefore, the measurement of quantum coherence can also quantify the amount of quantum correlation in a molecular magnetic system.

Influence of the external pressure. Recently, using Density Function Theory calculations [51], one of us showed that the application of an hydrostatic pressure in the prototype material KNaCuSi$_4$O$_{10}$ induces a structural contraction, which leads to a minimization of the degree of its quantum correlations [12]. Through the dependence of the magnetic coupling constant of the compound on the external pressure [12] we calculate magnetic susceptibilities, eq. (4), from each magnetic coupling constant. Thus, by using eq. (7) it is possible to evaluate the influence of an hydrostatic pressure on the quantum coherence of a low-dimensional molecular magnetic system. In this way, we establish a relationship between the quantum coherence and significant macroscopic effects, such as an external hydrostatic pressure applied on the magnetic material.

Figure 2 shows the temperature dependence of the quantum coherence for different values of hydrostatic pressure. As obtained in ref. [12], increasing the pressure in the system leads to a decrease on the lattice parameter and volume of unit cell; as a consequence, the exchange parameter of the system increases until it becomes positive changing the energy levels, i.e., the system ceases to be ordered antiferromagnetically in an entangled ground state $|01\rangle - |10\rangle / \sqrt{2}$ and is led to populate ferromagnetically ordered states with a lower degree of coherence. Due to this change of the exchange parameter sign, there is a gap in the coherence of the ground state, as can be seen in fig. 2; increasing the hydrostatic pressure on this prototype material leads to the decrease of the degree of coherence in the system.

Therefore, increasing the pressure changes the magnetic alignment, which yields a change in the occupation of the energy levels, leading the system to a less coherent configuration. In this context, it is possible to handle the degree
of coherence of a low-dimensional molecular magnetic system by managing the pressure applied on the system, since the external pressure induces a structural contraction in the metal-silicate framework, leading to a change of its magnetic alignment and reducing the degree of quantum coherence in the dimeric unit. This result shows that the degree of coherence in a spin cluster system can be controlled by the management of structural parameters such as the lattice parameter and volume of the unit cell, allowing the manipulation of the quantum coherence by materials engineering.

Influence of the longitudinal and transverse magnetic field. Unlike other quantum information theoretic quantifiers, $l_1$ norm quantum coherence is basis-dependent since it depends on the off-diagonal terms of the density matrix expressed in a reference basis, as can be seen from eq. (2). Thus, any density operator will be incoherent in its eigenbasis [17,27,34]; the reference basis $\{|k\}$ concerning the coherence is measured regarding the physical problem under investigation. For molecular magnetic systems, the standard reference basis for the density matrix is the spin eigenbasis in a particular direction, $\{S_x, S_y, S_z\}$, within a quantum metrology setting.

In order to investigate the influence of the application of an external magnetic field on the prototype material KNaCuSi$_{3}$O$_{10}$, we consider the magnetic field $\vec{B}$ along the $z$-direction. One can evaluate the coherence for two reference bases: one parallel to the applied field ($S_z$ eigenbasis) and another perpendicular to the field ($S_x$ or $S_y$ eigenbasis). The Hamiltonian that rules this system interacting with an external magnetic field is given by

$$\mathcal{H} = -J \vec{S}_1 \cdot \vec{S}_2 - \mu_B g \vec{B} \cdot (\vec{S}_1 + \vec{S}_2). \quad (9)$$

Thus, our aim is study how the applied fields, parallel to the density matrix basis $S_z$ (longitudinal field) and perpendicular to the density matrix basis $S_x$ (transverse field), affect the degree of quantum coherence in our prototype material.

1. Longitudinal field: The bipartite density matrix of this system can be written in the $S_z$ eigenbasis: $\{|00\}, \{|01\}, \{|10\}, \{|11\}\} \quad [43,44]$ as a X-shaped matrix:

$$\rho_z(T, B_z) = \frac{e^\beta}{2Z} \begin{pmatrix} 2e^{3\beta x} & 1 + e^{-4x} & 1 - e^{-4x} \\ 1 - e^{-4x} & 1 + e^{-4x} & 2e^{-\beta x} \end{pmatrix}, \quad (10)$$

where

$$Z(T, B_z) = e^x + e^{-3x} + 2e^x \cosh(\beta h_z), \quad (11)$$

with $\beta = 1/k_B T$, $x = \beta J/4$, $h_z = \mu_B g_z B_z$, and $Z$ is the partition function.

The trace norm quantum coherence, eq. (2), can be calculated in terms of these matrix elements as

$$C_z(T, B_z) = \frac{1 - e^{-4x}}{1 + e^{-4x} + 2 \cosh(\beta h_z)}. \quad (12)$$

Figure 3 shows the quantum coherence of our prototype material as a function of the applied longitudinal field (fig. 3(a)) and temperature (fig. 3(b)). As can be seen, the application of a longitudinal magnetic field decreases the degree of coherence. As a system in equilibrium at 0 K is always in its maximally entangled ground state $|01\rangle - |10\rangle/\sqrt{2}$, since it is an antiferromagnetic 1/2-spin dimer [12,36], when the longitudinal field reaches a critical value of $B_c = 21279$ Oe the system will be led to the incoherent ground state $|00\rangle$, i.e., all spins aligned with the applied field. Hence, there is an abrupt change in the degree of coherence of the ground state, the system changes from a maximally entangled ground state with $C_z = 1$ ($B < B_c$) to a completely incoherent ground state ($B \geq B_c$), due to the Zeeman effect along the parallel direction with the density matrix basis. Therefore, the application of a longitudinal magnetic field changes the energy eigenvalues, which leads the system to a different ground state with a smaller degree of coherence.

Although absolute zero is not physically realizable, the changes on the degree of coherence between the Cu(II) ions, due to the application of the longitudinal magnetic
field, are highlighted in low temperatures. At nonzero temperatures, the thermal fluctuations compete with the magnetic interactions changing the occupation of the energy levels [6,15,52]. Therefore, increasing the temperature will populate many incoherent states, decreasing the degree of coherence of the system. In contrast, when a high longitudinal magnetic field is applied at low temperatures, the ground state tends to be less coherent than some excited states. Thus, increasing the temperature may lead to a state with the highest degree of coherence, yielding a small increase on the quantum coherence, as can be seen in fig. 3(b) around 1 K. Similar effects were also encountered for the entanglement of formation and quantum discord in refs. [6,52–54].

2. Transverse field: On the other hand, the field applied on the z-direction breaks the isotropy of the Heisenberg interaction due to the Zeeman effect along this direction [1]. In this regard, in order to study the effects of the application of a transverse magnetic field on the quantum coherence of KNaCuSi$_4$O$_{10}$ compound, we rewrite the density matrix eq. (10) in the perpendicular eigenbasis, $S_x$, $\{|++\rangle, |+-\rangle, |-\rangle, |--\rangle\}$ as

\[
C_x(T, B_z) = \frac{e^x}{Z} \left( e^{2x} \sinh(\beta h_z) \cosh(\beta h_z) - 1 \right). \tag{13}
\]

In fig. 4, we show the quantum coherence of our metal-silicate framework as a function of the applied transverse field (fig. 4(a)) and temperature (fig. 4(b)). In contrast to the application of a longitudinal magnetic field (fig. 3), the transverse field increases and strengthens the degree of coherence between Cu(II) ions in the dimeric cluster. It also can be understood in terms of the population change of the ground state, due to the variation of the Boltzmann weights, which leads to a change on the occupation of the energy levels [6,15,52].

Due to the rotational invariance of the Bell states, at 0 K and $B_z < B_c$, the system is found in the maximally entangled ground state $\{|++\rangle, |+-\rangle\}/\sqrt{2}$, on the $S_x$ eigenbasis, with quantum coherence $C_x = 1$. For the transverse field $B_z \geq B_c$, the system will be led to the ground state $|0\rangle = \{(++\rangle + |+-\rangle + |-\rangle + |--\rangle)/2$, which has the maximal coherence degree $C_x = 3$, i.e., the ground state becomes maximally coherent beyond the coherence of the maximally entangled ground state, which shows that quantum coherence is a fundamental feature to indicate quantumness in an integral system far beyond quantum entanglement [17].

Therefore, the transition induced by the application of a transverse magnetic field describes an abrupt change in the degree of coherence of the ground state, due to the uncertainty relations between the $S_z$ spin direction of the Zeeman effect and the $S_z$ eigenbasis, in which the density matrix is written, eq. (13). This yields a change in the populations of the energy levels, leading the system to a state with the highest degree of coherence. Thus, unlike the longitudinal field, the transverse field effect is
to populate such coherent states, leading to an increase in the degree coherence of the system. This is a drastic difference from the quantum coherence in the parallel eigenbasis (fig. 3) and a signature of its basis dependence reported in the literature [17,27,34].

It is worth noting that, for $T > 20\, \text{K}$, the values of magnetic field needed to increase or decrease the coherence in this metal-silicate framework are higher than the available field intensities usually created in laboratories, which indicates that the coherence in this low-dimensional molecular magnetic system cannot be destroyed or enhanced by a common longitudinal or transverse magnetic field, respectively, for temperatures above $20\, \text{K}$, since the quantum coherence of this low-dimensional molecular magnetic system is resistant to magnetic field application above this temperature.

Conclusions. – In summary, we have shown a method to evaluate the degree of quantum coherence in low-dimensional magnetic materials composed of 1/2-spin dimers, where we investigate the influence of external parameters, such as temperature and magnetic fields, on the quantum coherence of the $\text{KNaCuSi}_2\text{O}_10$ prototype material, which is an ideal simulation of a two-qubit system. At zero magnetic field we associated the calculation of the trace norm quantum coherence with a magnetometric measurement of the magnetic susceptibility of the compound, using the experimental data reported in ref. [36], which characterizes the magnetic properties of this material. We established the theoretical relations between the measurement of quantum coherence and the thermodynamic properties of this prototype material, setting the path for the experimental measurement of quantum coherence in low-dimensional molecular magnetic materials.

In addition, we investigated the influence of the applied pressure on the degree of quantum coherence of our prototype material. We observed that increasing the external pressure yields a reduction of the degree of coherence in the system due to structural contraction provided by applying external pressure. Therefore, the quantum coherence of a molecular magnetic system can be handled by the management structural properties of the material. Moreover, we also presented a theoretical analysis of the influence of an external magnetic field on the degree of coherence of the system, where we investigated the basis dependence of the coherence. We found that when the longitudinal field is applied to the reference basis, it decreases the degree of coherence in the parallel eigenbasis, whereas if the transverse field is applied, it strengthens the degree of coherence between the Cu(II) ions in the dimeric cluster in the transverse eigenbasis.

In this context, the coherence of a low-dimensional molecular magnetic system can be handled by controlling the thermodynamics external parameters, such as temperature, external pressure and magnetic fields. These results offer an alternative way to identify quantum coherence in a condensed matter system, leading to promising applications in quantum information science such as the enhancement of quantum properties in low-dimensional molecular magnetic systems by materials engineering, and the development of novel candidate platforms for processing and transmission of quantum information.

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