Influence of hydrostatic pressure on the thermal entanglement of spins

C. S. Castro and M. S. Reis

Instituto de Física, Universidade Federal Fluminense

Av. Gal. Milton Tavares de Souza s/n, Gragoatá, 24210-346, Niterói, RJ, Brazil

K. Pirota

Instituto de Física Gleb Wataghin, Universidade Estadual de Campinas

Rua Sérgio Buarque de Holanda, 777, Cidade Universitária Zeferino Vaz, Barão Geraldo, 13083-859, Campinas, SP, Brazil

Abstract

Some thermodynamical properties of solids, such as magnetic susceptibility and heat capacity, can be used as entanglement witness. In this direction, some works have been using molecular magnets to investigate the thermal entanglement through experimental observation of magnetic susceptibility. The present work goes further and reports the influence of hydrostatic pressure on the thermal entanglement of spins. To this purpose we considered a dimer-trimer cluster and we verified that the entanglement of this set is strengthened due to an applied hydrostatic pressure of 5.7 kbar and 7.9 kbar.

Entanglement

Quantum states of composite systems can present nonlocal correlations among their parts [a]; and this nonlocality comes from an phenomenon named *entanglement*. A state ρ of N subsytems is defined to be not entangled if it can be written as a convex sum product states

$$\rho = \sum_j p_j \rho_1^j \otimes \cdots \otimes \rho_N^j,$$

where $\{p_j\}$ is the distribution of probabilities that satisfies $\sum_j p_j = 1$. In addition, $\{\rho_i^j\}$ is the density matrix that acts in the Hilbert spaces $\mathcal{H}_i$.

The entanglement present in the solids at finite temperature is named in the literature as *thermal entanglement*. This amazing phenomenon can be detected throught of an tool named *Entanglement Witness* (EW) [b]. An EW is a Hermitian operator which has negative values for entangled states; however, positive values do not guarantee separable states.

[a] A. Einstein, B. Podolsky, and N. Rosen, Phys. Rev. **47**, 777 (1935).
[b] M. Horodecki, P. Horodecki, and R. Horodecki, Phys. Lett. A, **23**, 1, (1996).

Note EW depends on the magnetic susceptibility and therefore it is not needed the full knowledge of the model Hamiltonian. The inequality below

$$\chi(T) = \frac{1}{3}\left(\chi^x(T) + \chi^y(T) + \chi^z(T)\right) \leq \frac{(g\mu_B)^2 NS}{3k_B T},$$

where S is the spin the particles and N is the number of the ions, leads to entanglement witness [a]:

$$EW(N) = \frac{3k_B T\chi(T)}{(g\mu_B)^2 NS} - 1.$$

If EW(N) $<$ 0 the system presents entanglement; however, EW(0) $>$ 0 does not necessarily implies separability.

[a] M. Wiesniak, V. Vedral, and C. Brukner, New J. Phys, 258 (2005).

The material - $Na_2Cu_5Si_{14}O_{14}$ compound

The aim of this work is to report an experimental observation of the thermal entanglement of $Na_2Cu_5Si_{14}O_{14}$ compound under hydrostatic pressure. The aim characteristics this compound are described below:

- It is composed by copper (s=1/2) separated in two groups containg two and three atoms each, and oxygen atoms.
- The zigzag chains of edge-charing square-planar CuO_4 is built throught the metal-oxygen connectivity.
- The chains are stacked obliquely in adjacents planes.
- The spins inside trimer are coupled antiferromagnetically with each other; the atoms of dimer interact ferromagnetically; the two sets of spins enteract antiferromagnatically with each other.

According to the exchange interactions between the spins (see the figure below), the Hamiltonian that describes this system is:

$$\mathcal{H} = -J_1\left(\vec{S}_1\cdot\vec{S}_2+\vec{S}_2\cdot\vec{S}_3\right)-J_2\left(\vec{S}_A\cdot\vec{S}_B\right)-J_3\left(\vec{S}_4\cdot\vec{S}_5\right)-g\mu_B\vec{H}\cdot\vec{S},$$

where $\vec{S}_A$ is the total spin of the dimer, $\vec{S}_B$ is the total spin of the trimer, $\vec{S}$ is the sum of $\vec{S}_A$ and $\vec{S}_B$, i.e., the total spin of the cluster. The Hamiltonian can be rewritten as

$$\begin{aligned}\mathcal{H} &= -\frac{J_1}{2}\left(S_B^2-S_{B'}^2-S_2^2\right)-\frac{J_2}{2}\left(S^2-S_A^2-S_B^2\right)\\ &\quad -\frac{J_3}{2}\left(S_A^2-S_4^2-S_5^2\right)-g\mu_B HS,\end{aligned}$$

where $S_{B'}=S_1+S_3$.

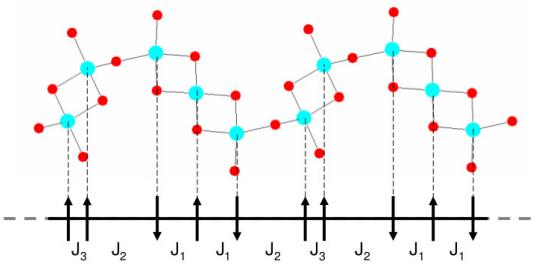

Figure: Top view of the structure of the $Na_2Cu_5Si_4O_{14}$ compound. The red smaller circles are the oxygen atoms and the blue larger circles are the copper atoms.

Magnetic behavior

Considering the van Vleck susceptibility and the eigenvalues of the last Hamiltonian, it is possible to obtain the theoritical magnetic susceptibility; and it is fitted to the experimental data (see the figure below).

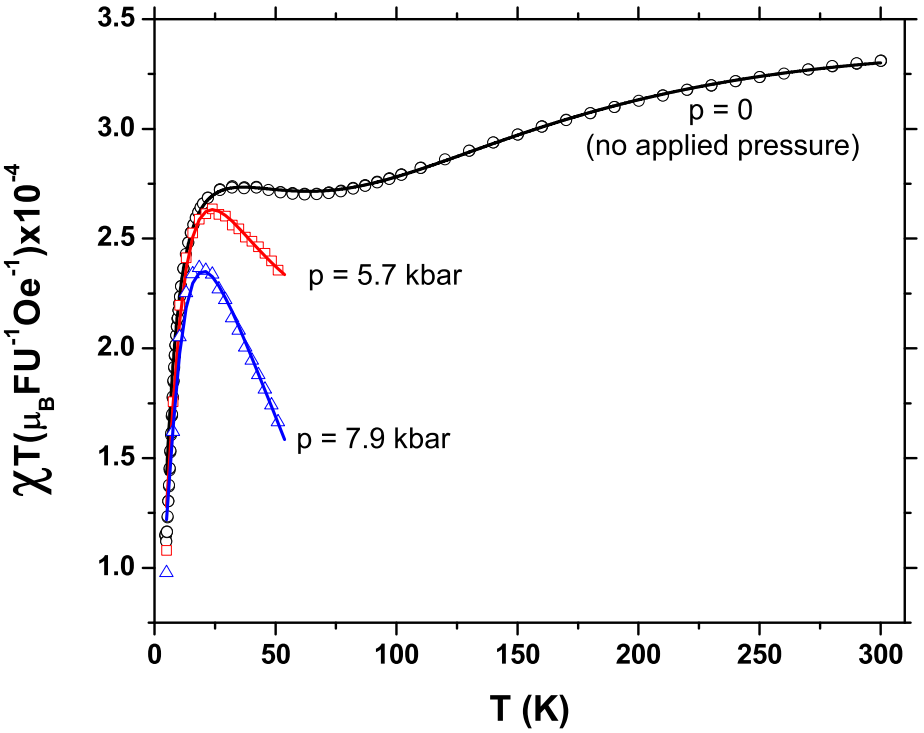

Figure: Magnetic susceptibility as function of temperature. The full lines are the theoretical predictions and the symbols represent the experimental data.

Unfortunetly, the magnetic signal of the cell is comparable to the sample for temperature above 100 K and therefore we present the experimental data only below 50 K. The parameters obtained fitting Van Vleck susceptibility to the experimental data are described below.

p (kbar)	J_1(K)	J_2(K)	J_3(K)	g	χ_{Ti} (μ_B/FU·Oe)
zero	-224.9	-8.01	40.22	2.23	$-4.99 \cdot 10^{-7}$
5.7	-123.98†	-11.08	40.83	2.55	$-2.24 \cdot 10^{-6}$
7.9	-109.92†	-11.35	337.02	2.64	$-4.89 \cdot 10^{-6}$

† These values are not reliable, since the susceptibility data is available only below 50 K.

Table: Parameters obtained fitting van Vleck susceptibility to the experimental data.

EW for different pressures

The figure below presents EW(2) and EW(5) under applied pressure. Note these quantities become farther away of EW $= 0$, i.e, the crossover point separating entangled and non-entangled states.

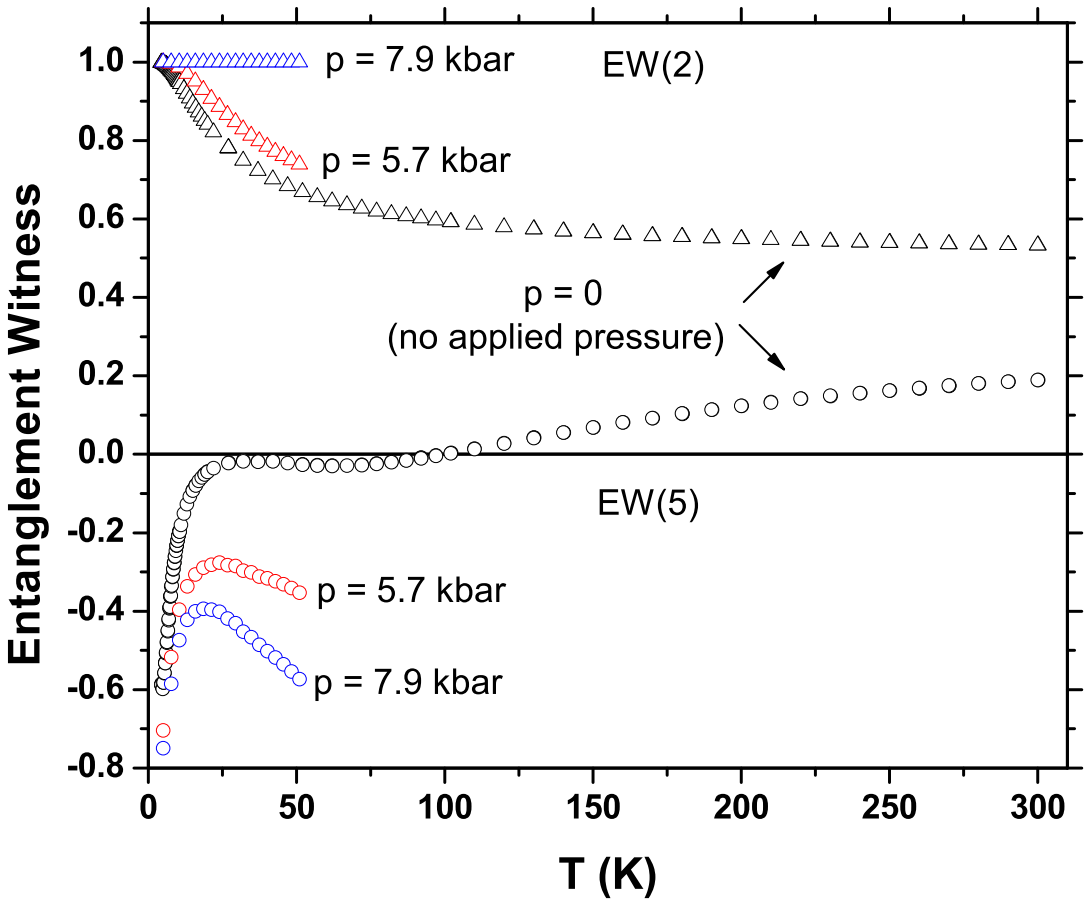

Figure: Entanglement witness for the system under different hydrostatic pressures.

EW at 50 K

It is possible to predict the range of pressure in which the system will present entanglement. The following figure shows that the lattice expansion would destroy the entangled states of the total system, not interesting from the applied point of view. On the other hand, a lattice contraction would bring to higher temperatures the entangled states; quite useful from the applied point of view.

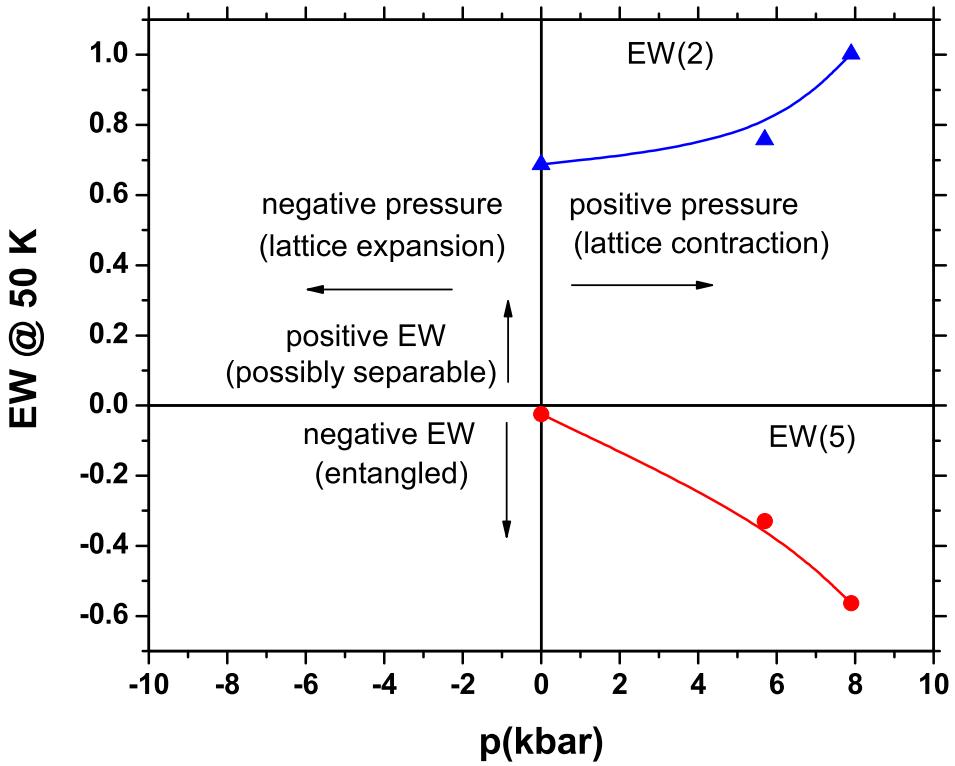

Figure: Entanglement witness as function the hydrostatic pressure for fixed temperature at 50 K for dimer system and total cluster.

Conclusions

In summary, we have established the presence of thermal entanglement in the compound $Na_2Cu_5Si_4O_{14}$ for differents hydrostatic pressure. We conclude that there is entanglement up to higher temperature in the system while the pressure increases. Furthermore, it is possible to predict which ranges of the pressure the system presents entanglement: lattice contraction. These results are notable since entanglement above room temperature constitute an useful tool for several tasks based on entanglement in their performance.

Acknowledgments

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