Entanglement of spin-1/2 Heisenberg antiferromagnetic quantum spin chains

Saulo Luis Lima da Silva

Abstract  The quantum entanglement measure is determined, for the first time, for a collection of spin-1/2 arranged in an infinite chain with finite temperature and applied to a single-crystal $\beta$-TeVO$_4$. The physical quantity proposed here to measure the entanglement is the distance between states by adopting the Hilbert–Schmidt norm. We relate the distance between states with the magnetic susceptibility. The decoherence temperature, above which the entanglement is suppressed, is determined for a system. A correlation among their decoherence temperatures and their respective exchange coupling constants is established; moreover, it is conjectured that the exchange coupling protects the system from decoherence as temperature increases.

Keywords  Entanglement · Quantum mechanics · Condensed matter · Magnetic materials · Quantum information

1 Introduction

Currently studying entanglement in condensed matter systems is of great interest. This interest stems from the fact that some behaviors of such systems can only be explained with the aid of entanglement. The magnetic susceptibility at low temperatures, quantum phase transitions, chemical reactions are examples where the entanglement is key ingredient for a complete understanding of the system. Furthermore, to produce a quantum processor, the entanglement of study condensed matter systems becomes essential. In condensed matter, the said magnetic materials are of particular interest. Among these we will study the antiferromagnetism which are described by Heisenberg model.

We use the Hilbert–Schmidt norm for measuring the distance between quantum states. The choice of this norm was due mainly to its application simplicity and strong geometric appeal. The question of whether this norm satisfies the conditions desirable for a good measure of entanglement was discussed in 1999 by Witte and Trucks [1]. They showed that the norm of Hilbert–Schmidt is not increasing under completely positive trace-preserving maps making use of the Lindblad theorem [2]. Ozawa argued that this norm does not satisfy this condition using an example of a completely positive map which can enlarge the Hilbert–Schmidt norm between two states [3]. However, this does not prove the fact that the entanglement measure based on the Hilbert–Schmidt norm is not entangled monotone.
This problem has come up in several contexts in recent years. Superselection structure of dynamical semigroups [4], entropy production of a quantum channel [5], condensed matter theory [6] and quantum information [7,19,24] are some examples. Several authors have been devoted to this issue in recent years [8–12] and other work on this matter is in progress by the author and collaborators.

The study of entanglement in Heisenberg chains is of great interest in physics and has been done for several years. In the early 2000s, O’Connor, Wootters, Wang and Zanardi showed how to get the density matrix of a chain of Heisenberg whose Hamiltonian commutes with the \( z \) component of the total spin [13,14]. Wieśniak, Vedral and Bruckner showed in 2005 how to relate entanglement with the magnetic susceptibility [15]. In 2008, Aldashin studied the entanglement in dimer systems [16]. The authors made use of Blaney and Bowers equation [17] to relate the entanglement with the magnetic susceptibility of the system. The entanglement of a dimer–trimer system was studied experimentally using magnetic susceptibility in 2008 by Souza et al. [18]. Del Cima et al. had in 2015 entanglement for the trimer compound, relating it to the magnetic susceptibility of the material. Also, obtained the entanglement depending on the temperature and the critical temperature of entanglement for two compounds that have not yet been studied in this respect [19].

In the present work, we have studied a Heisenberg infinite chain system from the perspective of entanglement. We can find a discussion of infinite chain in [13,15,20,32]. However, these discussions are limited to zero temperature or are not accurate results.\(^1\) In this paper, we have, accurately, detected entangled states in finite temperature. For this purpose, we make use of Bonner–Fisher model [21], and work of Eggert et al. [22], to relate the entanglement with the magnetic susceptibility of the system. In addition, we have, for the first time, an entanglement in the compound \( \beta\)-TeVO\(_4\). Present entanglement as a function of temperature as well as the critical temperature of entanglement.

The paper is structured as follows. In Sect. 2, we present the method we will use to quantify entanglement. In Sect. 3, we calculate the entanglement for a set of \( N \) particles arranged in a ring, after we will generalize this for an infinite chain. This result was applied to the \( \beta\)-TeVO\(_4\) compound. Finally, Sect. 4 is intended to conclusions.

2 Calculating the entanglement

Following [19], we consider a system that satisfies the Heisenberg Hamiltonian

\[
H = -J \sum_i S_i \cdot S_{i+1},
\]

where \( J \) is the exchange constant and \( S_i \) is the spin operator of the site \( i \). The Hamiltonian commutes with the \( z \)-component of total spin \([H, S^z] = 0\), there is no coherent superposition of states and \( J < 0 \). This allows us to write the reduced density matrix [13]

\[
\rho_{i,i+1} = \begin{pmatrix}
  v & 0 & 0 & 0 \\
  0 & w & z & 0 \\
  0 & z^* & w & 0 \\
  0 & 0 & 0 & v
\end{pmatrix},
\]

where the indices \( i \) and \( i + 1 \) refer to the site \( i \) and its nearest neighbor, respectively. We can relate the elements of the reduced density matrix with the correlation function per site as follows [14]:

\[
v = \frac{1}{4} + \langle S_i^z S_{i+1}^z \rangle.
\]

\(^{1}\) For use Entanglement Witnesses (EW).
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Fig. 1 Distance between states as a measure of entanglement

$$z = (S_i^x S_{i+1}^x) + (S_i^y S_{i+1}^y) + i(S_i^x S_{i+1}^y) - i(S_i^y S_{i+1}^x).$$ (4)

In the absence of an external magnetic field the system is isotropic; thus

$$z = 2(S_i S_{i+1}).$$ (5)

The system has the dimension of the Hilbert space associated $2 \otimes 2$. Therefore, we can use the criterion of Peres–Horodecki [23]. The eigenvalues of the partial transpose of $\rho_{i,i+1}$ are

$$\{w, w, v - |z|, v + |z|\}.$$ (6)

Hence, we can see that the system is entangled when

$$v < |z|,$$ (7)

otherwise, the system is separable.

Knowing what are the separate and entangled states, we can calculate how much each state is entangled. We use the Hilbert–Schmidt norm [1,24] to determine the distance between states to evaluate the degree of entanglement of the system. Let us consider a set $\Omega$ of all density matrices. It consists of two disjunctive subsets: the subset of separable states $\mathcal{S}$ and the subset of entangled states $\Sigma = \Omega - \mathcal{S}$. In this case, the entanglement is given by

$$\mathcal{E}(\rho_c) = \min_{\rho_s \in \mathcal{S}} D(\rho_s, \rho_c),$$ (8)

where $D$ is the distance between the density matrices $\rho_c$ (entangled) and the set of separable states $\mathcal{S}$ (see Fig. 1).

In other words, we take the degree of entanglement as the shortest distance between a given entangled state and the set of reduced density matrices separable. $\rho_s$ and $\rho_c$ will be given by

$$\rho_s = \begin{pmatrix} v_s & 0 & 0 & 0 \\ 0 & w_s & z & 0 \\ 0 & z^* & w_s & 0 \\ 0 & 0 & 0 & v_s \end{pmatrix}, \quad \text{and} \quad \rho_c = \begin{pmatrix} v_c & 0 & 0 & 0 \\ 0 & w_c & z & 0 \\ 0 & z^* & w_c & 0 \\ 0 & 0 & 0 & v_c \end{pmatrix}.$$ (9)

Hence, the entanglement is

$$\mathcal{E}(\rho_c) = \min \sqrt{\text{Tr}[(\rho_s - \rho_c)^2]} = 2 \min |v_s - v_c|.$$ (10)
It is easy to see that (10) is minimal when \( v_s = |z| \). Thus, the entanglement of the system is given by

\[
\mathcal{E}(\rho_e) = \max \left\{ 0, 2(|z| - v_e) \right\}. \tag{11}
\]

The term “\( \max \)” was introduced to avoid negative entanglement. Replacing (3) and (5) in (11), we obtain

\[
\mathcal{E}(\rho_e) = 2 \max \left[ 0, \left( 2|\langle S_i S_{i+1} \rangle| - \frac{1}{4} - \langle S_i S_{i+1} \rangle \right) \right]. \tag{12}
\]

Since the Hamiltonian \( H \) commutes with the spin component along the \( z \) direction, \( S_z \), one can show that the magnetic susceptibility along a given direction \( \alpha \) can be written as \[15\]

\[
\chi^\alpha(T) = \left( g \mu_B \right)^2 \frac{2}{k_B T} \left( \sum_{j,k=1}^{N} \langle S_j^\alpha S_k^\alpha \rangle - \left( \sum_{k=1}^{N} S_k^\alpha \right)^2 \right), \tag{13}
\]

and

\[
\chi(T) = \frac{\chi^x + \chi^y + \chi^z}{3}. \tag{14}
\]

It should be noticed that for optical lattices, the variance in (13) can be directly measured without to stand in need of the magnetic susceptibility \[25\].

If \( N \) is even, we have

\[
\langle S_i S_j \rangle_{\text{even}} = \frac{12k_B T \chi - 3N(g\mu_B)^2}{8(N-1)(g\mu_B)^2}, \tag{15}
\]

for \( N \) odd

\[
\langle S_i S_j \rangle_{\text{odd}} = \frac{12k_B T \chi - (3N-1)(g\mu_B)^2}{8(N-1)(g\mu_B)^2}, \tag{16}
\]

or

\[
\langle S_i S_j \rangle_{\text{odd}} = \langle S_i S_j \rangle_{\text{even}} + \frac{1}{8(N-1)}. \tag{17}
\]

Using (15), (16) and (12), we can relate the entanglement of the system of interest with the magnetic susceptibility of system. Note that \( \langle S_i S_j \rangle_{\text{odd}} = \langle S_i S_j \rangle_{\text{even}} \) when \( N \to \infty \).

### 3 Quantum correlations

Replacing (15) in (12), we have the entanglement for a ring with \( N \) even spins

\[
\mathcal{E}(\chi) = 2 \max \left[ 0, \left( 2 \left| \frac{12k_B T \chi - 3N(g\mu_B)^2}{8(N-1)(g\mu_B)^2} \right| - \frac{1}{4} \right) \right]. \tag{18}
\]
Similarly, replacing (16) in (12), we have the entanglement for a ring with \( N \) odd spins

\[
\mathcal{E}(\mathcal{X}) = 2 \max \left[ 0, \left( 2 \sqrt{\frac{12 k_B T \mathcal{X}^2 - (3N - 1)(g \mu_B)^2}{8(N - 1)(g \mu_B)^2}} - \frac{1}{4} \right) \right].
\]

(19)

In the limit \( N \to \infty \) the Eqs. (18) and (19) become equal.

In Ref. [21], Bonner and Fisher have shown that magnetic susceptibility for an infinite chain is

\[
\chi(T) = \frac{N(g \mu_B)^2(0.25 + 0.074795x + 0.075235x^2)}{k_B T(1.0 + 0.9931x + 0.172135x^2 + 0.757825x^3)},
\]

(20)

where \( x = |J|/k_B T \). In the low temperature regime, Eggert et al. [22] show an asymptotic dependence of the magnetic susceptibility with \((\ln T)^{-1}\). At high temperatures both results agree.

Taking the limit \( T \to 0 \) and replacing (20) in (19), we obtain the entanglement of an infinite chain at \( T = 0 \). In this case, using the susceptibility of Eggert et al. or of Bonner–Fisher give the same result

\[
\mathcal{E}(T = 0) = \frac{7}{16}.
\]

(21)

Note that this result is independent of \( J \). In other words, it is independent of the material. This result is significantly close to that found by O’Connor et al. [13], where the authors tried to answer the question about what extent each pair of nearest neighbors can be entangled. But we cannot say that the results found by them is optimal.

If we consider \( T > 0 \), at low temperature, we should use the result of Ref. [22]; but most of the materials in this temperature range undergoes phase transitions that prevent the use of the one-dimensional model. Fortunately, this temperature range is small (\( T < 5 \) K)! At high temperatures, we can use the result of Bonner and Fisher for thermal entanglement.

### 3.1 \( \beta \)-TcVO\(_4\) compound

Vanadium oxides with the \( V^{4+} \) ions (\( S = 1/2 \)) are excellent model systems for one-dimensional spin-1/2 quantum magnets. Its structure consists of zig-zag chains, as shown in Fig. 2. A simplified scheme of this structure can be seen in Fig. 3.

The interaction between nearest neighbors, represented by \( J_1 \), is weak in magnitude. Indeed, in Ref. [26], the authors have shown that in the temperature range of 5–130 K the interaction is dominated by \( J_2 \) and is of antiferromagnetic character, so \( |J_1| \ll |J_2| \). Therefore, we will take into account the interaction between next nearest neighbor represented for \( J_2 \) in Fig. 3. The interaction between the zig-zag chains \( J_\perp \), is also weak and will be neglected here. At low temperatures (\( T < 5 \) K), it features three different magnetics characteristics. This is due to unknown origin of phase transition and our model \( 1 - D \) is no longer very realistic. In short, in the temperature range of 5 K to 130K, we can consider this system as an infinite chain of spin-1/2 with antiferromagnetic interaction modeled by Heisenberg Hamiltonian (1).

The value found in [26] for the exchange interaction in this system is \( J/k_B = -21.4 \) K. Replacing it in (19) we obtain the thermal entanglement system and we found the critical temperature of entanglement. Figure 4 shows the entanglement as a function of temperature for this compound. This allows us to obtain materials with any critical temperature of entanglement previously desired. Thus, we are able to seek materials with appropriate \( J \), as already
was conjectured in [19]. This is outstandingly interesting for the study of processing and transmission of quantum information.

It is a difficult task to determine experimentally if a state is entangled or not. A widely used method for entanglement detection is the use of Entanglement Witnesses (EWs) [27, 28]. An observable $W$ can be used as an EW if $\text{Tr}(\rho W) < 0$, when $\rho$ is an entangled state. When $\text{Tr}(\rho W) \geq 0$, $\rho$ may or may not be entangled. Magnetic susceptibility was proposed as an EW [15], and several experimental results were obtained within this framework [18, 29–32]. At this point, it is easy to apply this method. Just do use the $\text{EW} = 6k_B T \left( \frac{\chi}{(g\mu_B)^2N} \right) - 1$ [15] and experimentally measured values of $\chi$ obtained in Ref. [26]. Thus, according to the definition of Entanglement Witness, the inequality $6k_B T \left( \frac{\chi}{(g\mu_B)^2N} \right) < 1$ determines the existence of entanglement. However, $6k_B T \left( \frac{\chi}{(g\mu_B)^2N} \right) \geq 1$ does not assure separability. This method reveals a critical temperature of $T \simeq 31 \text{ K}$. This show that some entangled

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**Fig. 2** (Color online) Crystal structure of $\beta$-TeV$_4$, viewed along $a$ (left) and $c$ (right) axis [26]

**Fig. 3** Schematic view of the interaction between the ions $V^{4+}$ in chain $\beta$-TeVO$_4$

**Fig. 4** Thermal entanglement compound $\beta$-TeVO$_4$. Modeled as an infinite chain of spin-1/2
states were not detected by the EW, since our previous results show entanglement in the system up to \( T \approx 47 \text{ K} \) (see Fig. 4).

Finally, this entanglement measure can be used to detect quantum phase transitions in Heisenberg chains with an external magnetic field and or anisotropy. In the present work, we study a Heisenberg model without external magnetic field and anisotropy. Therefore do not exhibit quantum phase transition. This is a task of a later study.

4 Conclusion

In conclusion, we have shown that an infinite chain entanglement spins has a nonzero value in both \( T = 0 \) and \( T > 0 \). The critical temperature of compound \( \beta\text{-TeVO}_4 \) was obtained. Calculations were obtained analytically, using the distance between states and the Hilbert–Schmidt norm as a measure of entanglement. Our results allow us to conclude that the critical temperature of entanglement increases directly with the increase in the exchange constant \( J \). This allows us to conclude that the exchange constant can be seen as a “shield” against decoherence of entanglement, due to increased temperature.

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