Quantum entanglement in trimer spin-1/2 Heisenberg chains with antiferromagnetic coupling

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The quantum entanglement measure is determined, for the first time, for antiferromagnetic trimer spin-1/2 Heisenberg chains. The physical quantity proposed here to measure the entanglement is the distance between states by adopting the Hilbert-Schmidt norm. The method is applied to the new magnetic Cu(II) trimer system, 2b.3CuCl$_2$.2H$_2$O, and to the trimuclear Cu(II) halide salt, (3MAP)$_2$Cu$_2$Cl$_8$. The decoherence temperature, above which the entanglement is suppressed, is determined for both systems. A correlation among their decoherence temperatures and their respective exchange coupling constants is established.

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I. INTRODUCTION

Since the seminal works by Einstein, Podolski and Rosen [1], and by Schrödinger [2], quantum entanglement has become one of the most amazing and pursued phenomenon in quantum mechanics, mainly, after the experiment realized by Aspect, Grangier and Roger [3]. During the last decade, quantum entanglement has been extremely important in processing and transmission of information [4, 5], in understanding the quantum phase transitions [6, 7], as well as in applications in quantum biology [8].

Very recently, an experimental realization of long-distance entanglement in antiferromagnetic spin chains has been performed [9]. However, in spite of being an old and deeply studied subject, from theoretical and experimental point of view, there still has a lack of a measure of entanglement – there is no quantitative method – a physical quantity which measures the degree of quantum entanglement. Qualitative criteria are available, where in some special cases, detect whether or not the entanglement is presented, without foresee how much a system is entangled. Since entanglement is a quantum mechanical phenomenon, it should not to be revealed at scales larger than atomic or in high temperatures, this is known as quantum decoherence. However, as it has been presented here, there are solids exhibiting quantum entanglement even at finite temperatures – the trimer spin-1/2 Heisenberg chain compounds with antiferromagnetic exchange coupling, 2b.3CuCl$_2$.2H$_2$O [10] and (3MAP)$_2$Cu$_2$Cl$_8$ [11]. As a physical quantity to measure quantum entanglement, use has been made of the distance between states [12, 13] by using the Hilbert-Schmidt norm [14].

The outline of this paper is as follows. In Section II, the method adopted to compute the quantum entanglement is introduced and its measure, the distance among states, is established for any spin-1/2 antiferromagnetic trimer. The quantum entanglement, for the compounds 2b.3CuCl$_2$.2H$_2$O and (3MAP)$_2$Cu$_2$Cl$_8$, and their critical temperatures, above which the entanglement vanishes, are computed and presented in Section III. Finally, Section IV is left for conclusions.

II. MEASURING THE QUANTUM ENTANGLEMENT

A antiferromagnetic trimer spin-1/2 Heisenberg chain can be represented by the Hamiltonian:

\[ H_{AF} = -J \sum_i \vec{S}_i \cdot \vec{S}_{i+1}, \]

where \( J < 0 \) is the exchange coupling constant and \( S_i \) is the spin operator for the \( i \)th spin (on site \( i \)). The Hamiltonian [11] commutes with the \( z \)-component of the total spin \( \langle S^2 \rangle \), \( [H_{AF}, S^2] = 0 \). Therefore, the reduced density matrix can be written as follows [15]:

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

such that the indices \( i \) and \( i+1 \) refer to the site \( i \), and its nearest neighbour site, \( i+1 \), respectively. Since there is no coherent superposition of states and the exchange coupling is antiferromagnetic, the density matrix [2] is rewritten as

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

The elements of the reduced density matrix [2] can be related with the correlation functions (per site) [16], and...
they read
\[ v = \frac{1}{4} + \langle S_i^x S_{i+1}^x \rangle, \quad z = \langle S_i^y S_{i+1}^y \rangle + i \langle S_i^z S_{i+1}^z \rangle - i \langle S_i^y S_{i+1}^x \rangle \]
and since \( \text{Tr}(\rho_{i,i+1}) = 1 \),
\[ w = \frac{1}{2}(1 - 2v). \]
However, the system is isotropic when in the absence of
external magnetic field, so
\[ v = \frac{1}{4} + \langle S_i S_{i+1} \rangle, \quad z = 2\langle S_i S_{i+1} \rangle, \]
\[ w = \frac{1}{4} - \langle S_i S_{i+1} \rangle. \]

Since the Hilbert space dimension is of a 2 \( \otimes \) 2-system,
\( \rho_{i,i+1} = (\rho^A \otimes \rho^B)_{i,i+1} \), the Peres-Horodecki criterion \( \text{[17]} \)
shall be used. The eigenvalues, \( \lambda_k = (\lambda_1, \lambda_2, \lambda_3, \lambda_4) \), of
the partial transposition of \( \rho_{i,i+1} \), are
\[ \lambda_k = (w, w, v + |z|, v - |z|). \] (8)
However, from (7) and (8), together to the fact that
\[ \langle S_i S_{i+1} \rangle = \frac{1}{2} \langle (S_i + S_{i+1})^2 \rangle - \frac{3}{4} \]
for \( T = 0K \), then,
\[ -\frac{3}{4} \leq \langle S_i S_{i+1} \rangle \leq -\frac{1}{4}, \]
which yields that \( \lambda_1 = \lambda_2 > 0 \) and \( \lambda_3 > 0 \). The Peres-Horodecki criterion states that, a system is entangled if, at least, one of the eigenvalues \( \lambda_k \) \( \text{[8]} \) is negative, otherwise, it is separable. It remains one eigenvalue to be
analysed, \( \lambda_4 = v - |z| \). Taking into account \( \text{[7]}, \text{[5]} \) and
\( \text{[10]} \), it stems that \( v < |z| \), which results \( \lambda_4 < 0 \), therefore,
as a consequence from the Peres-Horodecki criterion \( \text{[17]} \), the system is fully entangled for \( T = 0K \).
It shall be stressed that, from now on, by knowing the separate and the entangled states, it can calculated how
much a state is entangled. The distance between states
\( \text{[12]}, \text{[13]} \) has been adopted to measure the entanglement through the Hilbert-Schmidt norm \( \text{[14]} \). Therefore, the
entanglement measure is given by
\[ E(\rho) = \min D(\rho_t||\rho_e), \]
where \( D \) is the distance between separable and entangled states and, \( \rho_t \) and \( \rho_e \) are their reduced density matrices,
respectively. In other words, the entanglement is measured as the closest distance between a given entangled state and the set of separable states. The reduced density matrices, \( \rho_t \) and \( \rho_e \), associated to entangled and separable states, respectively, read
\[ \rho_e = \begin{pmatrix} v_\perp & 0 & 0 & 0 \\ 0 & w_\perp & z & 0 \\ 0 & z^* & w_\perp & 0 \\ 0 & 0 & 0 & v_\perp \end{pmatrix}, \]
and where the subscripts, \(< \) and \( \perp \), indicate that the condition, \( v < |z| \), is satisfied by the former and does not by
the latter – which should happen at finite temperatures, \( T > 0K \).

The measure of entanglement \( E(\rho) \) \( \text{[11]} \), by assuming the Hilbert-Schmidt norm \( \text{[14]} \), is now written as
\[ E(\rho) = E_0 \min \sqrt{\text{Tr}[(\rho_t - \rho_e)^2]} \]
\[ = 2E_0 \min |v_\perp - v_{\perp}|, \]
where \( E_0 \) is a normalization constant so that the entanglement measure \( \text{[14]} \) satisfies:
\[ 0 \leq E(\rho) \leq 1. \] (15)
Furthermore, \( E(\rho) \) \( \text{[14]} \) reaches its minimum for \( v_\perp = |z| \), giving rise to
\[ E(\rho) = E_0 \max \left[ 0, 2(|z| - v_{\perp}) \right], \]
where, in this case, \( E_0 = 1/4 \). Then, by substituting \( \text{[14]} \) in \( \text{[11]} \), it follows that
\[ E(\rho) = \]
\[ 2E_0 \max \left[ 0, \left( 2\langle S_i S_{i+1} \rangle - \frac{1}{4} - \langle S_i S_{i+1} \rangle \right) \right]. \] (17)

Due to the fact that the Hamiltonian \( H_{AF} \) \( \text{[11]} \) commutes with the spin component along the \( z \) direction \( S^z \), the magnetic susceptibility \( \text{[18]} \) along a given direction \( \alpha (\chi^\alpha(T)) \) can be written as
\[ \chi^\alpha(T) = \frac{(g\mu_B)^2}{k_B T} \sum_{i,j=1}^N \langle S_i^\alpha S_j^\alpha \rangle - \left( \sum_{i=1}^N S_i^\alpha \right)^2, \]
with
\[ \chi(T) = \chi^x + \chi^y + \chi^z, \]
being the average of the magnetic susceptibility measured along the three orthogonal axis. It should be noticed
that for optical lattices \( \text{[19]} \), the variances in \( \text{[18]} \) can be directly measured without to stand in need of the
magnetic susceptibility.

In the following Section, the quantum entanglement measure \( E(\rho) \) have been computed for the trimer compounds 2b.3CuCl$_2$.2H$_2$O \( \text{[14]} \) and (3MAP)$_2$.Cu$_2$.Cl$_8$ \( \text{[11]} \), and their respective entanglement critical temperatures determined.
III. QUANTUM ENTANGLEMENT MEASURE AND ANTIFERROMAGNETIC TRIMER SYSTEMS

Any antiferromagnetic trimer system, with exchange coupling constant $J$, as represented in Figure 1 can be modelled as proposed here. Despite there is also an exchange interaction among the trimers ($J_{\text{int}}$), such interaction is very small if compared with the intra-trimer exchange interaction ($J$), $J_{\text{int}} \ll J$, so it has not been taken into account. A general approach to calculate the quantum entanglement measure, $\mathcal{E}(\rho)$, has to be established before its further application for the compounds $2b.3\text{CuCl}_2.2\text{H}_2\text{O}$ [10] and (3MAP)$_2\text{Cu}_2\text{Cl}_8$ [11]. Bearing in mind [18] and [19], it straightly follows that

$$\chi(T) = \frac{2(g\mu_B)^2}{k_B T} (2(S_i S_{i+1}) + 1) ,$$

then

$$\chi(T) = \frac{2(g\mu_B)^2}{3k_B T} (2(S_i S_{i+1}) + 1) .$$

Therefore, from [21] and [17], the quantum entanglement measure $\mathcal{E}(\rho)$, reads

$$\mathcal{E}(\rho) = \mathcal{E}_0 \frac{k_B T}{(g\mu_B)^2} \max \left[ 0, \left( \frac{3}{2} \chi(T) - \frac{(g\mu_B)^2}{k_B T} \right) \right. \\
+ \left. \frac{(g\mu_B)^2}{2k_B T} - \frac{3}{2} \chi(T) \right] .$$

The mean susceptibility value $\chi(T)$ for the trimer system, with antiferromagnetic exchange coupling constant $J$, has been calculated by using the Van Vleck equation [20], yielding that

$$\chi(T) = \frac{(g\mu_B)^2}{4k_B T} \frac{1 + e^{\frac{J}{k_B T}} + 10e^{\frac{2J}{k_B T}}}{1 + e^{\frac{J}{k_B T}} + 2e^{\frac{2J}{k_B T}}} .$$

Finally, by substituting [23] in [22], the quantum entanglement measure ($\mathcal{E}(\rho)$) is attained as a function of the temperature ($T$) and the exchange coupling ($J$):

$$\mathcal{E}(J, T) = \mathcal{E}_0 \max \left[ 0, \left( \frac{3}{2} \chi(T) - \frac{(g\mu_B)^2}{k_B T} \right) \right. \\
+ \left. \frac{(g\mu_B)^2}{2k_B T} - \frac{3}{2} \chi(T) \right] .$$

with

$$\lim_{T \to 0} \mathcal{E}(J, T) = \frac{11}{8} \mathcal{E}_0 = \frac{11}{32} .$$

Moreover, in which concerns the result above [24], it should be stressed that the entanglement critical temperature ($T_c$) is defined as the one which vanishes identically the quantum entanglement measure, $\mathcal{E}(J, T)$:

$$\mathcal{E}(J, T)|_{T=T_c} = 0 .$$

Thus, for temperatures below the critical (decoherence) one, $T < T_c$, the system is entangled, whereas, for temperatures above it, $T \geq T_c$, the system experiences quantum decoherence, it assumes a separable state.

The application to any trimer system with antiferromagnetic interactions, in order to determinate the degree of entanglement (quantum entanglement measure) and the decoherence temperature (critical temperature) is now straightforward. The first material analysed was the new magnetic Cu(II) trimer system $2b.3\text{CuCl}_2.2\text{H}_2\text{O}$ [10], where $J/k_B = -20.0K$. The quantum entanglement measure, $\mathcal{E}(J, T)$ [24], of $2b.3\text{CuCl}_2.2\text{H}_2\text{O}$, as a function of temperature is displayed in Figure 2. The critical temperature obtained for $2b.3\text{CuCl}_2.2\text{H}_2\text{O}$, from solving [24] together with [25], is $T_c = 26.6K$. The second material analysed was a trimuclear Cu(II) halide

$^{1} b = \text{C}_6\text{H}_{11}\text{NO}_2$ (betaine). For details concerning crystal structure and magnetic properties, see [10].
The quantum entanglement measure, $\mathcal{E}(J, T)$ \cite{24}, of (3MAP)$_2$Cu$_2$Cl$_8$, as a function of temperature is presented in Figure 3, and its critical temperature (decoherence temperature), calculated in the same way as the first compound, is $T_c = 40, 2K$.

$\mathcal{E}(J, T)$ is proportional to $|J|$, $T_c \propto |J|$.

IV. CONCLUSIONS

The quantum entanglement is measured by the distance between states \cite{12,13}, through the Hilbert-Schmidt norm \cite{14}, and established for any spin-1/2 antiferromagnetic trimer. It is analytically computed for the new magnetic Cu(II) trimer system 2b.3CuCl$_2$.H$_2$O ($J/k_B = -20, 0K$) \cite{10}, and for the trinuclear Cu(II) halide salt (3MAP)$_2$Cu$_2$Cl$_8$ ($J/k_B = -30, 2K$) \cite{11}, as well as their decoherence (critical) temperatures, $T_c = 26, 6K$ and $T_c = 40, 2K$, respectively. Furthermore, the correlation among the decoherence temperature ($T_c$) and the absolute value of the exchange coupling constant ($|J|$), $T_c \propto |J|$, is explicitly identified – the greater $|J|$, the greater is $T_c$. It should be stressed that the quantum entanglement measure is independent on the exchange coupling only at $T = 0K$. Therefore, as a conjecture, the exchange coupling protects the system from decoherence as temperature increases.

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