Two Qubit Entanglement in $XYZ$ Magnetic Chain with DM Anisotropic Exchange Interaction

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In the present paper we study two qubit entanglement in the most general $XYZ$ Heisenberg magnetic chain with (non)homogeneous magnetic fields and the DM anisotropic antisymmetric exchange interaction, arising from the spin-orbit coupling. The model includes all known results as particular cases, for both antiferromagnetic and ferromagnetic $XX, XY, XXX, XXZ, XYZ$ chains. The concurrence of two qubit thermal entanglement and its dependence on anisotropic parameters, external magnetic field and temperature are studied in details. We found that in all cases, inclusion of the DM interaction, which is responsible for weak ferromagnetism in mainly antiferromagnetic crystals and spin arrangement in low symmetry magnets, creates (when it does not exist) or strengthens (when it exists) entanglement in $XYZ$ spin chain. This implies existence of a relation between arrangement of spins and entanglement, in which the DM coupling plays an essential role. It suggests also that anisotropic antisymmetric exchange interaction could be an efficient control parameter of entanglement in the general $XYZ$ case.

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I. INTRODUCTION

Entanglement property has been discussed at the early years of quantum mechanics as specifically quantum mechanical nonlocal correlation [1]–[3] and it becomes recently a key point of quantum information theory [4]. For entangled subsystems, the whole state vector cannot be separated into a product of the states of the subsystems, and the last ones are no longer independent even if they are far spatially separated. A measurement on one subsystem not only gives information about the other subsystem, but also provides possibilities of manipulating it. Therefore in quantum computations the entanglement becomes main tool of information processing, such as quantum cryptography, teleportation and etc.

For realizing quantum logic gates, several models have been proposed and demonstrated by experiments in cavity QED, ion trap, and NMR [5], [6]. Due to intrinsic pairwise character of the entanglement, in all these cases important is to find entangled qubit pairs. Generic two qubit state is characterized by $6$ real degrees of freedom. While separable two qubit state has only four degrees of freedom. It is clear that single qubit gates are unable to generate entanglement in an $N$ qubit system, because starting from separable state we will obtain another separable state with transformed by gates separable qubits. Then to prepare an entangled state one needs inter qubit interactions which is a two qubit gate. The well known example of two qubit gate generating entanglement is Controlled Not (CNOT) gate [7]. Moreover realization of two qubit controlled gates is a necessary requirement for implementation of the universal quantum computa-

This interaction arises from extending the Anderson’s theory of superexchange interaction by including the spin orbit coupling effect [12] , and it is important not only for
weak ferromagnetism but also for the spin arrangement in antiferromagnets of low symmetry. In the present paper we show that the Dzialoshinsky-Moriya interaction plays an essential role for entanglement of two qubits in magnetic spin chain model of most general XYZ form. We find that in all cases, inclusion of the DM interaction creates (when it does not exist) or strengthens (when it exists) entanglement. In particular case of isotropic Heisenberg XXZ model discussed above, inclusion of this term increases entanglement for antiferromagnetic case and even in ferromagnetic case, for sufficiently strong coupling \( D > (kT \sinh^{-1} |\lambda|/kT - J^2)^{1/2} \), it creates entanglement. These results imply existence of an intimate relation between weak ferromagnetism of mainly antiferromagnetic crystals and the spin arrangement in antiferromagnets of low symmetry, with entanglement of spins. Moreover it shows that the DM interaction could be an efficient control parameter of entanglement in the general XYZ model.

II. XYZ HEISENBERG MODEL

The Hamiltonian of XYZ model for \( N \) qubits is

\[
H = \sum_{i=1}^{N-1} \frac{1}{2} \left[ J_\sigma \sigma_i^x \sigma_{i+1}^x + J_y \sigma_i^y \sigma_{i+1}^y + J_z \sigma_i^z \sigma_{i+1}^z \right] + (B + b) \sigma_i^z + (B - b) \sigma_i^z + \vec{D} \cdot \left( \vec{\sigma}_i \times \vec{\sigma}_{i+1} \right)
\]

where \( B, b \)- external homogeneous and nonhomogeneous magnetic fields respectively, the last term is the DM coupling. Choosing \( \frac{\vec{D}}{2} = \frac{\vec{D}}{2} \cdot \vec{z} \) the Hamiltonian for two qubits becomes

\[
H = \frac{1}{2} \left[ J_\sigma \sigma_1^x \sigma_2^x + J_y \sigma_1^y \sigma_2^y + J_z \sigma_1^z \sigma_2^z \right] + (B + b) \sigma_1^z + (B - b) \sigma_2^z + D(\sigma_1^z \sigma_2^z - \sigma_1^y \sigma_2^y)
\]

and in the matrix form

\[
H = \begin{bmatrix}
\frac{J_\sigma}{2} + B & 0 & 0 & \frac{J_z - J_y}{2} \\
0 & \frac{J_\sigma}{2} + b & J_\sigma + J_y + iD & 0 \\
0 & -J_\sigma + J_y - iD & -\frac{J_z}{2} - b & 0 \\
\frac{J_z - J_y}{2} & 0 & 0 & \frac{J_z}{2} - B
\end{bmatrix}
\]

To study thermal entanglement firstly we need to obtain all the eigenvalues and eigenstates of the Hamiltonian \( H \): \( H|\Psi_i\rangle = E_i|\Psi_i\rangle \), \( i = 1, 2, 3, 4 \). The eigenvalues (energy levels) are:

\[
E_1 = \frac{J_\sigma}{2} - \mu \quad E_2 = \frac{J_\sigma}{2} + \mu \quad E_3 = -\frac{J_\sigma}{2} - \nu \quad E_4 = -\frac{J_\sigma}{2} + \nu
\]

where \( \frac{J_\sigma - J_y}{2} = J_- \), \( \frac{J_\sigma + J_y}{2} = J_+ \), \( \mu = \sqrt{B^2 + J_y^2} \), \( \nu = \sqrt{b^2 + J_x^2 + D^2} \) and corresponding wave functions are:

\[
|\Psi_1\rangle = \frac{1}{\sqrt{2(\mu^2 + \nu^2)}} \begin{bmatrix} J_- \ 0 \ 0 \ -(B + \mu) \end{bmatrix}
\]

\[
|\Psi_2\rangle = \frac{1}{\sqrt{2(\mu^2 + \nu^2)}} \begin{bmatrix} J_- \ 0 \ 0 \ -(B - \mu) \end{bmatrix}
\]

\[
|\Psi_3\rangle = \frac{-i}{\sqrt{2(\mu^2 + \nu^2)}} \begin{bmatrix} 0 \ J_+ + iD \ 0 \ -(b + \nu) \end{bmatrix}
\]

\[
|\Psi_4\rangle = \frac{1}{\sqrt{2(\mu^2 + \nu^2)}} \begin{bmatrix} 0 \ J_+ + iD \ 0 \ -(b - \nu) \end{bmatrix}
\]

For \( B = 0, b = 0, D = 0 \) the wave functions reduce to the Bell states

\[
|\Psi_2\rangle \rightarrow |B_0\rangle = \frac{1}{\sqrt{2}} (|00\rangle + |11\rangle)
\]

\[
|\Psi_4\rangle \rightarrow |B_1\rangle = \frac{1}{\sqrt{2}} (|01\rangle + |10\rangle)
\]

\[
|\Psi_3\rangle \rightarrow |B_2\rangle = \frac{1}{\sqrt{2}} (|01\rangle - |10\rangle)
\]

\[
|\Psi_1\rangle \rightarrow |B_3\rangle = \frac{1}{\sqrt{2}} (|00\rangle - |11\rangle)
\]

The state of the system at thermal equilibrium is determined by the density matrix

\[
\rho(T) = \frac{e^{-H/kT}}{Tr[e^{-H/kT}]} = \frac{e^{-H/kT}}{Z},
\]

where \( Z \) is the partition function, \( k \) is Boltzmann’s constant and \( T \) is the temperature. Then for Hamiltonian \( H \) we find

\[
e^{-H/kT} = I + \frac{(-H/kT)}{1!} + \frac{(-H/kT)^2}{2!} + \cdots + \frac{(-H/kT)^n}{n!} + \cdots
\]

\[
e^{-H/kT} = \begin{bmatrix}
A_{11} & 0 & 0 & A_{14} \\
0 & A_{22} & A_{23} & 0 \\
0 & A_{32} & A_{33} & 0 \\
A_{41} & 0 & 0 & A_{44}
\end{bmatrix}
\]
where
\[ A_{11} = -e^{\frac{\mu}{kT}} \left[ \cosh \frac{\mu}{kT} - \frac{B}{\mu} \sinh \frac{\mu}{kT} \right] \]
\[ A_{14} = -e^{\frac{\lambda}{kT}} J \frac{\mu}{\sinh \frac{\mu}{kT}} \]
\[ A_{22} = e^{\frac{\nu}{kT}} \left[ \cosh \frac{\nu}{kT} - \frac{b}{\nu} \sinh \frac{\nu}{kT} \right] \]
\[ A_{23} = -e^{\frac{J_z}{kT}} J \sinh \frac{\nu}{kT} \]
\[ A_{32} = -e^{\frac{J_z}{kT}} J \sinh \frac{\nu}{kT} \]
\[ A_{33} = e^{\frac{J_z}{kT}} \left[ \cosh \frac{\nu}{kT} + \frac{b}{\nu} \sinh \frac{\nu}{kT} \right] \]
\[ A_{41} = -e^{\frac{\lambda}{kT}} J \frac{\mu}{\sinh \frac{\mu}{kT}} \]
\[ A_{44} = e^{\frac{\lambda}{kT}} \left[ \cosh \frac{\mu}{kT} + \frac{B}{\mu} \sinh \frac{\mu}{kT} \right] \] (9)
and
\[ Z = Tr[e^{-H/kT}] = 2 \left[ e^{\frac{\mu}{kT}} \cosh \frac{\mu}{kT} + e^{\frac{\lambda}{kT}} \cosh \frac{\nu}{kT} \right]. \]

As \( \rho(T) \) represents a thermal state, the entanglement in this state is called the thermal entanglement. The concurrence \( C \) (the order parameter of entanglement) is defined as [17],
\[ C = \max \{ \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4, 0 \} \] (10)
where \( \lambda_i \) (i = 1, 2, 3, 4) are the ordered square roots of the eigenvalues of the operator
\[ \rho_{12} = \rho(\sigma^y \otimes \sigma^y) \rho^*(\sigma^y \otimes \sigma^y) \] (11)
and \( \lambda_1 > \lambda_2 > \lambda_3 > \lambda_4 > 0 \). The concurrence is a bounded function \( 0 \leq C \leq 1 \). When the concurrence \( C = 0 \), states are unentangled; when \( C = 1 \), states are maximally entangled. In our case:
\[ \lambda_{1,2} = e^{\frac{\lambda}{kT}} \frac{1 + \frac{J_z}{\mu} \sinh \frac{\mu}{kT} \pm \frac{J_z}{\mu} \cosh \frac{\mu}{kT}}{Z} \] (12)
\[ \lambda_{3,4} = e^{\frac{\lambda}{kT}} \frac{1 + \frac{J_z^2 + D^2}{\nu^2} \sinh \frac{\nu}{kT} \pm \frac{J_z^2 + D^2}{\nu} \cosh \frac{\nu}{kT}}{Z} \]
where \( \mu \equiv \sqrt{B^2 + J_z^2}, \nu \equiv \sqrt{b^2 + J_z^2 + D^2} \). Before calculating the concurrence for the general XYZ case (Section 7) it is instructive to consider particular reductions of XYZ model and compare corresponding concurrences with known results.

**III. ISING MODEL**

Let \( J_x = J_y = 0 \) and \( J_z \neq 0 \) and the Hamiltonian is
\[ H = \frac{1}{2} \left( J_z \sigma_x^z \sigma_y^z + (B + b) \sigma_x^z + (B - b) \sigma_y^z + D(\sigma_x^x \sigma_y^x - \sigma_x^y \sigma_y^y) \right) \]
The eigenvalues are
\[ \lambda_{1,2} = \frac{e^{-J_z/kT}}{Z} \] (13)
\[ \lambda_{3,4} = \frac{e^{\lambda/kT}}{Z} \frac{1 + \frac{D^2}{\nu^2} \sinh \frac{\nu}{kT} \pm \frac{D}{\nu} \cosh \frac{\nu}{kT} \pm \frac{J_z^2 + D^2}{\nu} \cosh \frac{\nu}{kT}}{Z} \]
where \( \mu = B, \nu = \sqrt{\nu^2 + D^2} \) and
\[ Z = Tr[e^{-H/kT}] = 2 \left[ e^{-\mu/kT} \cosh \frac{\mu}{kT} + e^{\lambda/kT} \cosh \sqrt{\nu^2 + D^2} \right]. \]

**A. Pure Ising Model \( (B = 0, b = 0, D = 0) \)**

1. **Antiferromagnetic Case \( (J_z > 0) \):**

The ordered eigenvalues are
\[ \lambda_1 = \lambda_2 e^{J_z/2kT} \frac{Z}{Z} \] (14)
where \( Z = 4 \cosh \frac{J_z}{kT} \) and the concurrence is
\[ C_{12} = \max \left\{ -e^{-J_z/2kT} \frac{Z}{2 \cosh \frac{J_z}{kT}}, 0 \right\} = 0 \] (15)
and there is no entanglement.

2. **Ferromagnetic Case \( (J_z < 0) \):**

The ordered eigenvalues are
\[ \lambda_1 = \lambda_2 e^{-J_z/2kT} \frac{Z}{Z} \] (16)
where \( Z = 4 \cosh \frac{J_z}{kT} \) and the concurrence is
\[ C_{12} = \max \left\{ -e^{-|J_z|/2kT} \frac{Z}{2 \cosh \frac{|J_z|}{kT}}, 0 \right\} = 0 \] (17)
It means that in both antiferromagnetic and ferromagnetic cases there is no entanglement in pure Ising Model for any \( T \).

**B. Ising Model with Homogeneous Magnetic Field \( (B \neq 0, b = 0, D = 0) \)**

The ordered eigenvalues are
\[ \lambda_1 = \lambda_2 e^{J_z/2kT} \frac{Z}{Z} , \quad \lambda_3 = \lambda_4 = e^{-J_z/2kT} \frac{Z}{Z} \] (18)
where \( Z = 2 \left[ e^{-J_z/2kT} \cosh \frac{B}{kT} + e^{J_z/2kT} \cosh \frac{B}{kT} \right] \) and the concurrence
\[ C_{12} = \max \left\{ -e^{-J_z/2kT} \frac{Z}{2 \cosh \frac{B}{kT}}, 0 \right\} = 0 \] (19)
and there is no entanglement.

**C. Ising Model with Nonhomogeneous Magnetic Field \( (B = 0, b \neq 0, D = 0) \)**

The concurrence is
\[ C_{12} = \max \left\{ -e^{-J_z/2kT} \frac{Z}{2 \cosh \frac{b}{kT}}, 0 \right\} = 0 \] (20)
and there is no entanglement.

As we can see in pure Ising model and including homogeneous (B) and nonhomogeneous (b) magnetic fields no entanglement occurs [19, 20, 21].
D. Ising Model with DM Coupling

\((B = 0, b = 0, D \neq 0)\)

The eigenvalues are
\[
\begin{align*}
\lambda_1 &= \frac{e^{(J_z+2D)/2kT}}{Z} , \quad \lambda_2 = \frac{e^{-(J_z-2D)/2kT}}{Z} \quad (21) \\
\lambda_3 &= \lambda_4 = \frac{e^{-J_z/2kT}}{Z} . \quad (22)
\end{align*}
\]

where \(Z = 2 \left[ e^{|D|/2kT} \cosh \frac{D}{kT} + e^{-|J_z|/2kT} \right] . \)

1. Antiferromagnetic Case \((J_z > 0)\):

Ordering the eigenvalues \(\lambda_1 > \lambda_2 > \lambda_3 = \lambda_4\) we have the concurrence
\[
C_{12} = \max \left\{ \sinh \frac{|D|}{kT} - e^{-|J_z|/2kT}, 0 \right\} . \quad (23)
\]

Then \(C_{12} = 0\) (no entanglement) if \(\sinh \frac{|D|}{kT} \leq e^{-|J_z|/2kT}\). When \(\sinh \frac{|D|}{kT} > e^{-|J_z|/2kT}\) the states are entangled
\[
C_{12} = \sinh \frac{|D|}{kT} - e^{-|J_z|/2kT} \cosh \frac{|D|}{kT} + e^{-|J_z|/2kT} . \quad (24)
\]

Moreover states become more entangled for low temperatures: maximally entangled for any \(D\) and \(T = 0\) so that \(\lim_{T \to 0} C_{12} = 1\) and for stronger DM coupling \(\lim_{D \to \infty} C_{12} = 1\). With \(T\) growing, \(D_{\min} = kT \sinh^{-1} e^{-|J_z|/kT}\) is growing so that we need to increase \(D\) to have entangled states.

2. Ferromagnetic Case \((J_z < 0)\):

a) With weak DM coupling \(|D| < |J_z|\) there is no entanglement Ordering the eigenvalues \(\lambda_3 = \lambda_4 > \lambda_1 > \lambda_2\) we have the concurrence
\[
C_{12} = \max \left\{ -\cosh \frac{|D|}{kT} e^{-|J_z|/kT} + e^{J_z/2kT}, 0 \right\} = 0 . \quad (25)
\]

b) With strong DM coupling \(|D| > |J_z|\) Ordering the eigenvalues \(\lambda_1 > \lambda_3 = \lambda_4 > \lambda_2\) and we have the concurrence
\[
C_{12} = \max \left\{ \sinh \frac{|D|}{kT} - e^{J_z/2kT}, 0 \right\} . \quad (26)
\]

Then \(C_{12} = 0\) (no entanglement) if \(\sinh \frac{|D|}{kT} \leq e^{J_z/2kT}\). When \(\sinh \frac{|D|}{kT} > e^{J_z/2kT}\) or \(|D| > |J_z| + \frac{kT}{2} \ln(1 + e^{-J_z/2kT})\) the states are entangled
\[
C_{12} = \sinh \frac{|D|}{kT} - e^{J_z/2kT} \cosh \frac{|D|}{kT} + e^{J_z/2kT} . \quad (27)
\]

Moreover states become more entangled for low temperatures \(\lim_{T \to 0} C_{12} = 1\) and for stronger DM coupling \(\lim_{D \to \infty} C_{12} = 1\). As we can see there is entanglement even in ferromagnetic case with sufficiently strong DM coupling. Comparison of (23) and (27) shows that in anti-ferromagnetic case, states can be more easily entangled then in the ferromagnetic one

IV. XX HEISENBERG MODEL

For \(J_x = 0, J_z = J_y \equiv J\), the Hamiltonian is
\[
H = \frac{1}{2} \left[ J (\sigma_1^x \sigma_2^x + \sigma_1^y \sigma_2^y) + (B+b) \sigma_1^z + (B-b) \sigma_2^z + D (\sigma_1^x \sigma_2^y - \sigma_1^y \sigma_2^x) \right] .
\]

The eigenvalues are
\[
\begin{align*}
\lambda_{1,2} &= \frac{1}{Z} \left[ \sqrt{1 + \frac{J^2 + D^2}{\nu^2}} \sinh \frac{\nu}{kT} + \sqrt{J^2 + D^2} \sinh \frac{1}{kT} \right] , \quad (28)
\end{align*}
\]

where \(\nu = \sqrt{J^2 + b^2 + D^2}\) and
\[
Z = \text{Tr}[e^{-H/kT}] = 2 \left[ \cosh \frac{B}{kT} + \cosh \frac{\nu}{kT} \right] .
\]

A. Pure XX Heisenberg Model \((B = 0, b = 0, D = 0)\)

The eigenvalues are
\[
\lambda_1 = \frac{e^{J/kT}}{Z} , \quad \lambda_2 = \lambda_3 = \frac{1}{Z} , \quad \lambda_4 = \frac{e^{-J/kT}}{Z} . \quad (29)
\]

1. Antiferromagnetic Case \(J > 0\)

The ordered eigenvalues are \(\lambda_1 > \lambda_2 > \lambda_3 > \lambda_4\) and the concurrence is
\[
C_{12} = \max \{ \sinh \frac{J}{kT} - 1, 0 \} \quad \text{so that}
\]
\[
\lim_{T \to 0} C_{12} = 1 . \quad (30)
\]

2. Ferromagnetic Case \(J < 0\)

He eigenvalues are
\[
\lambda_1 = \frac{e^{-|J|/kT}}{Z} , \quad \lambda_2 = \lambda_3 = \frac{1}{Z} , \quad \lambda_4 = \frac{e^{J/kT}}{Z} . \quad (31)
\]

\(\lambda_4 > \lambda_2 = \lambda_3 > \lambda_1\) and the concurrence is
\[
C_{12} = \max \{ \sinh \frac{|J|}{kT} - 1, 0 \} \quad \text{and}
\]
\[
a) \sinh \frac{|J|}{kT} > 1 \Rightarrow C_{12} = \frac{\sinh \frac{|J|}{kT} - 1}{\cosh \frac{|J|}{kT} + 1} . \quad (32)
\]
b) $\sinh \frac{|j|}{kT} \leq 1 \Rightarrow C_{12} = 0$ no entanglement for

$$T > \frac{|j|}{k} [\sinh^{-1} 1]^{-1}$$  \hspace{1cm} (33)$$

In both cases states are entangled at sufficiently small temperature $T < T_C = \frac{|j|}{k} [\sinh^{-1} 1]^{-1}$.

**B. XX Heisenberg Model with Magnetic Field**

$(B \neq 0, b = 0, D = 0)$

The eigenvalues are

$$\lambda_1 = e^{j/kT} \frac{Z}{Z}, \ \lambda_2 = \lambda_3 = 1, \ \lambda_4 = e^{-j/kT} \frac{Z}{Z}. \hspace{1cm} (34)$$

where

$$Z = 2 \left[ \cosh \frac{B}{kT} + \cosh \frac{J}{kT} \right]. \hspace{1cm} (35)$$

and the concurrence is $C_{12} = \max \{ \sinh \frac{j}{kT} - 1 \ cosh \frac{kT}{j} + \cosh \frac{kT}{j}, 0 \}$ and

a) $\sinh \frac{|j|}{kT} > 1 \Rightarrow C_{12} = \frac{\sinh \frac{j}{kT} - 1}{\cosh \frac{kT}{j} + \cosh \frac{kT}{j}}$

b) $\sinh \frac{|j|}{kT} \leq 1, \ C_{12} = 0$ no entanglement for

$$T > \frac{|j|}{k} [\sinh^{-1} 1]^{-1}$$  \hspace{1cm} (36)

It shows that inclusion of magnetic field does not change the critical temperature for concurrence in both antiferromagnetic and ferromagnetic cases. Pairwise entanglement in N-qubit XX chain and experimental realization of XX model has been discussed in [3, 6, 18, 22] and [23].

**C. XX Heisenberg Model with DM Coupling**

$(B = b = 0, \ D \neq 0)$

The eigenvalues are

$$\lambda_1 = \frac{e^{-\beta/kT}}{Z}, \ \lambda_2 = \frac{e^{-\beta/kT}}{Z}, \ \lambda_3 = \frac{e^{\beta/kT}}{Z}, \ \lambda_4 = \frac{e^{-\beta/kT}}{Z}.$$

where $\beta > 0$, $\beta = \sqrt{J^2 + D^2}$ and $Z = 2 (1 + \cosh \frac{\beta}{kT})$. The ordered eigenvalues are $\lambda_4 > \lambda_3 > \lambda_1 = \lambda_2$ and the concurrence is

$$C_{12} = \max \{ \sinh \frac{j}{kT} - 1 \ cosh \frac{kT}{j} + \cosh \frac{kT}{j}, 0 \} \hspace{1cm} (38)$$

where $\nu = \sqrt{J^2 + D^2}$ :

a) $\sinh \frac{|j|}{kT} > 1 \Rightarrow C_{12} = \frac{\sinh \frac{j}{kT} - 1}{\cosh \frac{kT}{j} + \cosh \frac{kT}{j}}$

b) $\sinh \frac{|j|}{kT} \leq 1 \Rightarrow C_{12} = 0$ there is no entanglement.

Entanglement increases with growth of DM coupling in both anti-ferromagnetic and ferromagnetic cases.

**V. XY HEISENBERG MODEL**

For $J_x = 0, J_y \neq J_y$, the Hamiltonian is

$$H = \frac{1}{2}[J_x \sigma_x^1 \sigma_x^2 + J_y (\sigma_y^1 \sigma_y^2 + (B+b) \sigma_z^1 + (B-b) \sigma_z^2 + D(\sigma_x^1 \sigma_x^2 - \sigma_y^1 \sigma_y^2)]]$$

The eigenvalues are

$$\lambda_{1,2} = \frac{1}{Z} \left[ \sqrt{1 + \frac{J_x^2}{\mu^2} \sinh^2 \frac{\mu}{kT} \sinh^2 \frac{\mu}{kT}} \right], \hspace{1cm} (39)$$

$$\lambda_{3,4} = \frac{1}{Z} \left[ \sqrt{1 + \frac{J_x^2 + D^2}{\nu^2} \sinh^2 \frac{\nu}{kT} \sinh^2 \frac{\nu}{kT}} \right], \hspace{1cm} (40)$$

where $\mu = \sqrt{B^2 + J_x^2}$, $\nu = \sqrt{b^2 + D^2 + J_y^2}$, $J_{\pm} = \frac{J_x + J_y}{2}$

and

$$Z = Tr[e^{-H/kT}] = 2 \left[ \cosh \frac{\mu}{kT} + \cosh \frac{\nu}{kT} \right]. \hspace{1cm} (41)$$

**A. Pure XY Heisenberg Model** $(B = 0, b = 0, D = 0)$

The eigenvalues are

$$\lambda_1 = \frac{e^{-j/kT}}{Z}, \ \lambda_2 = \frac{e^{-j/kT}}{Z}, \ \lambda_3 = \frac{e^{j/kT}}{Z}, \ \lambda_4 = \frac{e^{-j/kT}}{Z}.$$

where

$$Z = 2 \left[ \cosh \frac{J}{kT} + \cosh \frac{J_y}{kT} \right]. \hspace{1cm} (42)$$

For $J_x = J(1 + \gamma)$ and $J_y = J(1 - \gamma)$ so that $J_+ = J, J_- = J\gamma$, the eigenvalues are

$$\lambda_1 = \frac{e^{j/\gamma/kT}}{Z}, \ \lambda_2 = \frac{e^{-j/\gamma/kT}}{Z}, \ \lambda_3 = \frac{e^{j/kT}}{Z}, \ \lambda_4 = \frac{e^{-j/kT}}{Z}. \hspace{1cm} (43)$$

1. **Anti-ferromagnetic Case $J_x > 0$ and $J_y > 0$**

The ordered eigenvalues are $\lambda_3 > \lambda_1 > \lambda_2 > \lambda_4$ and the concurrence

$$C_{12} = \max \{ \sinh \frac{j}{kT} - \cosh \frac{j}{kT}, 0 \} \hspace{1cm} (44)$$

a) $\sinh \frac{|j|}{kT} > \cosh \frac{|j|}{kT} \Rightarrow C_{12} = \sinh \frac{j}{kT} - \cosh \frac{j}{kT}, \hspace{1cm} (lim_{T \rightarrow 0} C_{12} = 1)$

b) $\sinh \frac{|j|}{kT} \leq \cosh \frac{|j|}{kT} \Rightarrow C_{12} = 0$ there is no entanglement.

In Fig. 1, we plot the concurrence $C_{12}$ in XY Heisenberg antiferromagnet as function of $J_+ \frac{1}{kT}$ and $\frac{J}{kT}$. 


2. Ferromagnetic Case $J_x < 0$ and $J_y < 0$

$$C_{12} = \max \left\{ \sinh \frac{J_x}{kT} - \cosh \frac{J_y}{kT}, 0 \right\}$$

a) $\sinh \frac{J_x}{kT} > \cosh \frac{J_y}{kT}$

$$C_{12} = \frac{\sinh \frac{J_x}{kT} - \cosh \frac{J_y}{kT}}{\cosh \frac{J_x}{kT}} + \cosh \frac{J_y}{kT}$$

$$\lim_{T \to 0} C_{12} = 1$$

b) $\sinh \frac{J_x}{kT} \leq \cosh \frac{J_y}{kT} \Rightarrow C_{12} = 0$ there is no entanglement.

In Fig. 2, we plot the concurrence $C_{12}$ in XY Heisenberg ferromagnet as function of $\frac{J_x}{kT}$ and $\frac{J_y}{|J_z|}$.

FIG. 2: Concurrence $C_{12}$ in XY ferromagnet as function of $\frac{J_x}{kT}$ and $\frac{J_y}{|J_z|}$.

The eigenvalues are

$$\lambda_1 = \frac{e^{J_x/kT}}{Z}, \quad \lambda_2 = \frac{e^{-J_x/kT}}{Z}$$

$$\lambda_3 = \frac{e^{\sqrt{J_x^2 + D^2}/kT}}{Z}, \quad \lambda_4 = \frac{e^{-\sqrt{J_x^2 + D^2}/kT}}{Z}$$

where

$$Z = 2 \left[ \cosh \frac{J_x}{kT} + \cosh \frac{\sqrt{J_x^2 + D^2}}{kT} \right]$$

1. Antiferromagnetic Case

It shows that for any temperature $T$ we can adjust sufficiently strong DM coupling $D$ to have entanglement.

a) $\sinh \frac{\sqrt{J_x^2 + D^2}}{kT} > \cosh \frac{J_y}{kT} \Rightarrow$

$$C_{12} = \frac{\sinh \frac{\sqrt{J_x^2 + D^2}}{kT} - \cosh \frac{J_y}{kT}}{\cosh \frac{\sqrt{J_x^2 + D^2}}{kT}} + \cosh \frac{J_y}{kT}$$

b) $\sinh \frac{\sqrt{J_x^2 + D^2}}{kT} \leq \cosh \frac{J_y}{kT} \Rightarrow C_{12} = 0$ there is no entanglement.

2. Ferromagnetic Case

Ferromagnetic case gives the same result as antiferromagnetic case. Comparison with pure XY model [9] and [11] shows that level of entanglement is increasing with growing DM coupling $D$ and $C_{12} = 1$ when $D \to \infty$.

VI. XXX HEISENBERG MODEL

For $J_x = J_y = J_z \equiv J$, the Hamiltonian is

$$H = \frac{1}{2} [J (\sigma_1^x \sigma_2^x + \sigma_1^y \sigma_2^y + \sigma_1^z \sigma_2^z) + (B + b) \sigma_1^z]$$

$$+ (B - b) \sigma_2^z + D (\sigma_1^x \sigma_2^y - \sigma_1^y \sigma_2^x)]$$

The eigenvalues are

$$\lambda_{1,2} = \frac{e^{-J/2kT}}{Z}$$

$$\lambda_{3,4} = \frac{e^{J/2kT}}{Z} \sqrt{1 + \frac{J^2 + D^2}{k^2} \sinh^2 \frac{\nu}{kT} + \frac{J^2 + D^2}{\nu} \sinh \frac{\nu}{kT}}$$

where

$$Z = 2 \left[ e^{-J/2kT} \cosh \frac{B}{kT} + e^{J/2kT} \cosh \frac{\sqrt{J^2 + b^2 + D^2}}{kT} \right]$$
A. Pure XXX Model \((B = 0, b = 0, D = 0)\)

The eigenvalues are
\[
\lambda_{1,2} = \frac{e^{-J/2kT}}{Z}, \quad \lambda_3 = \frac{e^{-J/2kT}}{Z}, \quad \lambda_4 = \frac{e^{3J/2kT}}{Z}
\]
where
\[
Z = 2 \left[ e^{-J/2kT} + e^{J/2kT} \cosh \frac{J}{kT} \right]
\] (55)

1. Antiferromagnetic case \((J > 0)\):

The concurrence is
\[
C_{12} = \max \left\{ -\frac{\cosh \frac{J}{kT}}{\cosh \frac{J}{kT} + e^{J/2kT}}, 0 \right\}
\] (57)
a) \(\sinh \frac{J}{kT} > e^{-J/kT}\)
\[
C_{12} = \frac{\sinh \frac{J}{kT} - e^{-J/kT}}{e^{-J/2kT} + \cosh \frac{J}{kT}}
\] (58)

For sufficiently small temperature \(T < \frac{2J}{k \ln 3}\) entanglement occurs and \(\lim_{T \to 0} C_{12} = 1\)

b) \(\sinh \frac{J}{kT} \leq e^{-J/kT} \Rightarrow C_{12} = 0\) there is no entanglement.

2. Ferromagnetic case \((J < 0)\):

The concurrence is
\[
C_{12} = \max \left\{ -\frac{\cosh \frac{|J|}{kT}}{\cosh \frac{|J|}{kT} + e^{|J|/2kT}}, 0 \right\}
\] (59)

C. XXX Heisenberg Model with DM Coupling \((B = 0, b = 0, D \neq 0)\)

The eigenvalues are
\[
\lambda_{1,2} = \frac{e^{-J/2kT}}{Z}, \quad \lambda_3 = \frac{e^{(J-2\sqrt{J^2+D^2})/2kT}}{Z}, \quad \lambda_4 = \frac{e^{(J+2\sqrt{J^2+D^2})/2kT}}{Z}
\] (60)

1. Antiferromagnetic Case \((J > 0)\):

The concurrence is
\[
C_{12} = \max \left\{ \frac{\sin \sqrt{\frac{J^2+D^2}{kT}}}{\sin \sqrt{\frac{J^2+D^2}{kT}} + e^{-J/kT}}, 0 \right\}
\] (61)
a) \(\sin \sqrt{\frac{J^2+D^2}{kT}} > e^{-J/kT}\)
\[
C_{12} = \frac{\sin \sqrt{\frac{J^2+D^2}{kT}} - e^{-J/kT}}{e^{-J/2kT} + \sin \sqrt{\frac{J^2+D^2}{kT}}}
\] (62)

For a given temperature, when
\[
D > \sqrt{kJT\sinh^{-1}e^{-J/kT} - J^2}
\] (63)
there is entanglement.

b) \(\sin \sqrt{\frac{J^2+D^2}{kT}} \leq e^{-J/kT}\)
\[
C_{12} = 0 \text{ there is no entanglement.}
\] (64)

2. Ferromagnetic Case \((J < 0)\):

The concurrence is
\[
C_{12} = \max \left\{ \frac{\sin \sqrt{\frac{J^2+D^2}{kT}}}{\sin \sqrt{\frac{J^2+D^2}{kT}} + e^{-J/kT}}, 0 \right\}
\] (65)
a) \(\sin \sqrt{\frac{J^2+D^2}{kT}} < e^{-J/kT}\)
\[
C_{12} = \frac{\sin \sqrt{\frac{J^2+D^2}{kT}} - e^{-J/kT}}{e^{-J/2kT} + \sin \sqrt{\frac{J^2+D^2}{kT}}}
\] (66)

For a given temperature, when
\[
D > \sqrt{kJT\sinh^{-1}e^{-J/kT} - J^2}
\] (67)
there is entanglement.

b) \(\sin \sqrt{\frac{J^2+D^2}{kT}} \leq e^{-J/kT}\)
\[
C_{12} = 0 \text{ there is no entanglement.}
\] (68)
For a given temperature, when
\[ D > \sqrt{kT \sinh^{-1} |J|/kT - J^2} \] (70)
there is entanglement.

b) \( \sinh \frac{\sqrt{J^2 + D^2}}{kT} < e^{\frac{|J|}{kT}} \Rightarrow C_{12} = 0 \)

As we can see inclusion of DM coupling \( D \) in XXX case increases entanglement in antiferromagnetic case and even create entanglement in ferromagnetic case. Thermal entanglement and entanglement teleportation in XXX Heisenberg chain with DM interaction has been studied in [3].

VII. XXZ HEISENBERG MODEL

For \( J_x = J_y = J \neq J_z \) the Hamiltonian is
\[
H = \frac{1}{2} \left[ J(\sigma_i^x \sigma_i^x + \sigma_i^y \Delta \sigma_i^z \sigma_i^z) + (B + b) \sigma_i^z \right] + (B - b) \sigma_i^z + D(\sigma_i^x \sigma_i^y - \sigma_i^y \sigma_i^x) \] (71)
where \( \Delta \equiv J_z/J \). The eigenvalues are

\[
\lambda_{1,2} = \frac{\mp 1}{Z} \left[ 1 + \frac{J^2 + D^2}{2\nu^2} \sinh^2 \frac{\nu}{kT} + \frac{\sqrt{J^2 + D^2}}{\nu} \sinh \frac{\nu}{kT} \right] \] (72)

\[
\lambda_{3,4} = \frac{\mp 1}{Z} \sqrt{1 + \frac{J^2 + D^2}{\nu^2} \sinh^2 \frac{\nu}{kT} + \frac{\sqrt{J^2 + D^2}}{\nu} \sinh \frac{\nu}{kT}} \] (73)

where \( \mu = B, \nu = \sqrt{J^2 + D^2 + B^2} \) and

\[
Z = 2 \left[ e^{-J_z/2kT} \cosh \frac{B}{kT} + e^{J_z/2kT} \cosh \frac{\nu}{kT} \right] \]

A. Pure XXZ Heisenberg Model

\( (B = 0, b = 0, D = 0) \)

In this case the eigenvalues become

\[
\lambda_{1,2} = \frac{e^{-J_z/2kT}}{Z}, \quad \lambda_3 = \frac{e^{(J_z - 2J)/2kT}}{Z}, \quad \lambda_4 = \frac{e^{(J_z + 2J)/2kT}}{Z} \] (74)

where \( \beta = J \) and \( Z = 2 \left[ e^{-J_z/2kT} + e^{J_z/2kT} \cosh \frac{J_z}{kT} \right] \).

1. Antiferromagnetic Case \( (J > 0) \):

For \( |\Delta| < 1 \) weak anisotropy (\( \Delta > 0 \) easy axis, \( \Delta < 0 \) easy plane) and \( \Delta > 1 \) strong anisotropy, the concurrence is

\[
C_{12} = \max \left\{ \sinh \frac{J_z}{kT} - e^{-J_z/kT}, 0 \right\} \] (75)

a) \( \sinh \frac{J_z}{kT} > e^{-J_z/kT} \)

\[
C_{12} = \sinh \frac{J_z}{kT} - e^{-J_z/kT} \] (81)

where

\[
Z = 2 \left[ e^{-J_z/2kT} + e^{J_z/2kT} \cosh \frac{\sqrt{J^2 + D^2}}{kT} \right] \]

b) \( \sinh \frac{J_z}{kT} \leq e^{-J_z/kT} \Rightarrow C_{12} = 0, \) no entanglement.

From above formulas follow that for sufficiently small temperature \( T \) the states are entangled.

For \( \Delta \leq -1 \) the concurrence is

\[
C_{12} = \max \left\{ \frac{-\cosh \frac{|J|}{kT}}{\cosh \frac{|J|}{kT} + e^{J_z/kT}}, 0 \right\} = 0 \] (82)

and no entanglement.

For \( \Delta = 1 \) the anisotropic model reduces the isotropic XXX model, and the concurrence reduces to

\[
C_{12} = \max \left\{ \frac{e^{2J_z/kT} - 3}{e^{2J_z/kT} + 3}, 0 \right\} = 0 \] (83)

When the temperature is larger than the critical temperature \( T_C = \frac{2J}{\kappa \ln 3} \) the thermal entanglement disappears.

2. Ferromagnetic Case \( (J < 0) \):

For \( \Delta < 1 \) The concurrence is

\[
C_{12} = \max \left\{ \sinh \frac{|J|}{kT} - e^{J_z/kT}, 0 \right\} \] (84)

a) \( \sinh \frac{|J|}{kT} > e^{J_z/kT} \)

\[
C_{12} = \sinh \frac{|J|}{kT} - e^{J_z/kT} \] (85)

b) \( \sinh \frac{|J|}{kT} \leq e^{J_z/kT} \Rightarrow C_{12} = 0 \)

For \( \Delta \geq 1 \) the concurrence is

\[
C_{12} = \max \left\{ \frac{-\cosh \frac{|J|}{kT}}{\cosh \frac{|J|}{kT} + e^{J_z/kT}}, 0 \right\} = 0 \] (86)

and no entanglement.

B. XXZ Heisenberg Model with DM Coupling

\( (B = 0, b = 0, D \neq 0) \)

The eigenvalues are

\[
\lambda_{1,2} = \frac{e^{-J_z/2kT}}{Z}, \quad \lambda_3 = \frac{e^{(J_z - 2\sqrt{J^2 + D^2})/2kT}}{Z} \] (87)

\[
\lambda_4 = \frac{e^{(J_z + 2\sqrt{J^2 + D^2})/2kT}}{Z} \] (88)

where

\[
Z = 2 \left[ e^{-J_z/2kT} + e^{J_z/2kT} \cosh \frac{\sqrt{J^2 + D^2}}{kT} \right] \]

and no entanglement.
1. Antiferromagnetic case \((J > 0)\):

The concurrence is

\[
C_{12} = \max \left\{ \frac{\sinh \frac{\sqrt{J^2 + D^2}}{kT} - e^{-J_z/kT}}{\cosh \frac{\sqrt{J^2 + D^2}}{kT} + e^{-J_z/kT}}, 0 \right\}
\]  
(84)

\(a)\) \(\sinh \frac{\sqrt{J^2 + D^2}}{kT} > e^{-J_z/kT}\)

\[
C_{12} = \frac{\sinh \frac{\sqrt{J^2 + D^2}}{kT} - e^{-J_z/kT}}{\cosh \frac{\sqrt{J^2 + D^2}}{kT} + e^{-J_z/kT}}
\]  
(85)

and entanglement increases with growing \(D\).

Entanglement for XXZ Heisenberg model was considered in [29] and effect of \(D\) interaction on XXZ model in [32].

VIII. XYZ HEISENBERG MODEL

A. Pure XYZ Model \((B = 0, b = 0, D = 0)\)

The eigenvalues are

\[
\lambda_1 = e^{\frac{(J_x - 2J_z)}{2kT}}, \quad \lambda_2 = e^{\frac{(J_x + 2J_z)}{2kT}},
\]

\[
\lambda_3 = e^{\frac{(J_y - 2J_z)}{2kT}}, \quad \lambda_4 = e^{\frac{(J_y + 2J_z)}{2kT}}
\]

where

\[
Z = 2 \left[ e^{-J_z/2kT} \cosh \frac{J_y}{kT} + e^{J_z/2kT} \cosh \frac{J_y}{kT} \right]
\]

(86)

1. Antiferromagnetic Case :

\(J_z > J_y > J_x > 0 \Rightarrow J_z > 0, J_x = |J_x| < 0, J_y = |J_y| < 0.\) The biggest eigenvalue is \(\lambda_4 = \frac{(J_x + 2J_z)}{2Z}\) and the concurrence is

\[
C_{12} = \max \left\{ \frac{\sinh \frac{J_y}{kT} - \cosh \frac{J_x}{kT} e^{-J_z/kT}}{\cosh \frac{J_y}{kT} + \cosh \frac{J_x}{kT} e^{-J_z/kT}}, 0 \right\}
\]

(87)

Then entanglement occurs when

\[
f(T) = \sinh \frac{J_y}{kT} - \cosh \frac{J_x}{kT} e^{-J_z/kT} > 0.
\]

(88)

2. Ferromagnetic Case :

\(J_y > J_x > J_z > 0 \Rightarrow J_y > 0, J_x = |J_x| < 0, J_z = |J_z| < 0\). The biggest eigenvalue is

\[
\lambda_1 = e^{\frac{(J_y + 2J_z)}{2kT}}
\]

and the concurrence is

\[
C_{12} = \max \left\{ \frac{\sinh \frac{J_y}{kT} - \cosh \frac{J_x}{kT} e^{-J_z/kT}}{\cosh \frac{J_y}{kT} + \cosh \frac{J_x}{kT} e^{-J_z/kT}}, 0 \right\}
\]

(89)

Then entanglement occurs when

\[
f(T) = \sinh \frac{J_y}{kT} - \cosh \frac{J_x}{kT} e^{-J_z/kT} > 0.
\]

(90)

FIG. 3: Concurrence in XYZ antiferromagnet as function of \(T\)

This formula shows that entanglement increases with lowering temperature. In Fig. 3, we plot function \(f(T)\) for \((J_x, J_y, J_z) = (3, 2, 1)\). It shows entanglement for \(T < T_c\). In addition, from [30] we have entanglement increasing with growing anisotropy \(J_+\) and decreasing with growing anisotropy \(J_-\). Moreover it increases with growing \(J_+\).

FIG. 4: Concurrence in XYZ ferromagnet as function of \(T\)

\((J_x, J_y, J_z) = (-3, -2, -1)\). It shows that entanglement increases with growing anisotropy \(J_+\) and decreases with growing anisotropy \(J_-\). Moreover it increases with growing \(J_+\). Thermal entanglement in pure XYZ model has been studied in [31], [32]. Enhancement of entanglement in XYZ model in the presence of an external magnetic field considered in [33] and influence of intrinsic decoherence on quantum teleportation in [34].
B. **XYZ Model with Magnetic Field**

\( (B = 0, b = 0, D = 0) \)

The full anisotropic XYZ Heisenberg spin two-qubit system in which a magnetic field is applied along the z-axis, was studied by Zhou et al. The enhancement of the entanglement for particular fixed magnetic field by increasing the \( z \)-component of the coupling coefficient between the neighboring spins, was their main finding.

C. **XYZ Model with DM Coupling**

\( (B = 0, b = 0, D \neq 0) \)

\[
\lambda_1 = \frac{e^{(-J_z+2J_\perp)/2kT}}{e^{(-J_z+2J_\perp)/2kT} + \nu} \quad \lambda_2 = \frac{e^{(-J_z-2J_\perp)/2kT}}{e^{(-J_z-2J_\perp)/2kT} + \nu} \quad \lambda_3 = \frac{\nu}{e^{(-J_z+2J_\perp)/2kT} + \nu} \quad \lambda_4 = \frac{\nu}{e^{(-J_z-2J_\perp)/2kT} + \nu}
\]

where \( \nu = \sqrt{J_z^2 + D^2} \)

\[
Z = 2 \left[ e^{-J_z/2kT} \cosh \frac{J_z}{kT} + e^{J_z/2kT} \cosh \frac{\nu}{kT} \right]
\]

1. **Antiferromagnetic Case** :

The concurrence is

\[
C_{12} = \max \{ \sinh \frac{\nu}{kT} - \frac{e^{J_z/kT} \cosh \frac{J_z}{kT}}{\sinh \frac{\nu}{kT} + e^{-J_z/kT} \cosh \frac{J_z}{kT}}, 0 \} \quad (95)
\]

and entanglement occurs when

\[
\sinh \frac{\sqrt{J_z^2 + D^2}}{kT} > e^{-J_z/kT} \cosh \frac{J_z}{kT}
\]

In Fig. 5, we plot the concurrence \( C_{12} \) as function of \( D \) and \( T \). Comparing with pure XYZ case (90), we find that inclusion of DM coupling increases entanglement.

2. **Ferromagnetic Case** :

The concurrence is

\[
C_{12} = \max \{ \sinh \frac{\nu}{kT} - \frac{e^{J_z/kT} \cosh \frac{J_z}{kT}}{\sinh \frac{\nu}{kT} + e^{-J_z/kT} \cosh \frac{J_z}{kT}}, 0 \} \quad (96)
\]

and entanglement occurs for sufficiently strong \( D \)

\[
\sinh \frac{\sqrt{J_z^2 + D^2}}{kT} > e^{-J_z/kT} \cosh \frac{J_z}{kT}
\]

Fig. 6, shows \( C_{12} \) as function of \( D \) and \( T \).

Fig. 6: Concurrence \( C_{12} \) in XYZ ferromagnet as function of \( D \) and \( T \).

FIG. 5: Concurrence \( C_{12} \) in XYZ antiferromagnet as function of \( D \) and \( T \).
was found that the DM interaction can excite the entanglement and teleportation fidelity. As was noticed DM interaction could be significant in designing spin-based quantum computers [34]. Moreover, studying the effect of a phase shift on amount transferable two-spin entanglement in a spin chain [35], it was shown that maximum attainable entanglement enhanced by DM interaction.

Therefore would be interesting to consider most general XY/Z Heisenberg models with DM interaction as quantum channel for quantum teleportation which requires to know dependence of pairwise entanglement on the number of qubits in the spin chain. These questions now are under investigation.

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