Effect of an uniaxial single-ion anisotropy on the quantum and thermal entanglement of a mixed spin-$\frac{1}{2}, S$ Heisenberg dimer

Hana Vargová$^a$, Jozef Strečka$^b$, Natália Tomášovičová$^a$

$^a$Institute of Experimental Physics, Slovak Academy of Sciences, Watsonova 47, 040 01 Košice, Slovakia
$^b$Department of Theoretical Physics and Astrophysics, Faculty of Science, P. J. Šafárik University, Park Angelinum 9, 040 01 Košice, Slovakia

Abstract

Exact analytical diagonalization is used to study the bipartite entanglement of the antiferromagnetic mixed spin-$(1/2, S)$ Heisenberg dimer (MSHD) with the help of negativity. Under the assumption of uniaxial single-ion anisotropy affecting higher spin-$S$ $(S > 1/2)$ entities only, the ground-state degeneracy $2S$ is partially lifted and the ground state is two-fold degenerate with the total magnetization per dimer $\pm (S - 1/2)$. It is shown that the largest quantum entanglement is reached for the antiferromagnetic ground state of MSHD with arbitrary half-odd-integer spins $S$, regardless of the exchange and single-ion anisotropies. Contrary to this, the degree of a quantum entanglement in MSHD with an integer spin $S$ for the easy-plane single-ion anisotropy, exhibits an increasing tendency with an obvious spin-$S$ driven crossing point. It is shown that the increasing spin magnitude is a crucial driving mechanism for an enhancement of a threshold temperature above which the thermal entanglement vanishes. The easy-plane single-ion anisotropy together with an enlargement of the spin-$S$ magnitude is other significant driving mechanism for an enhancement of the thermal entanglement in MSHD.

Keywords: Heisenberg dimer, bipartite entanglement, exact diagonalization

1. Introduction

One of the most fascinating feature of quantum mechanical systems is an entanglement, referred to non-local correlations among the system constituents. A discovery of its importance in a quantum information processing [1] has initiated an intensive investigation of this unconventional phenomenon in various quantum systems. From the application point of view there naturally arises a question how to stabilize an entanglement at non-zero (ideally room) temperature, because an entanglement is rapidly reduced through thermal fluctuations. The Heisenberg dimer represents a profound theoretical model for analysing the bipartite entanglement, because its mathematical simplicity and quantum nature merge together. It was elucidated during last several years, that the implementation of additional stimuli, like non-uniform magnetic field, seems to be a relevant mechanism for an accrument of entanglement stability [2-6]. Another mechanism for an enhancement of entanglement lies in an anisotropy of a quantum system like the exchange anisotropy [3, 5, 7-10], Dzyaloshinskii-Moriya anisotropy [4, 8, 9] or diversity of spin parity [8, 11, 12]. Although all aforementioned mechanisms may enlarge the threshold temperature, they unfortunately simultaneously reduce a strength of the entanglement. Inspired by the findings of Solano-Carrillo et al. [13, 14], which imply that the uniaxial single-ion anisotropy may enhance the degree of thermal entanglement, we will investigate the simultaneous effect of an uniaxial single-ion anisotropy and the spin magnitude on a bipartite entanglement of MSHD.

2. Model and Method

Let us consider MSHD consisting of two different spins defined through the Hamiltonian

$$\hat{H} = J \left( \Delta (\hat{\mu}^i \hat{S}^x + \hat{\mu}^j \hat{S}^y) + \hat{\mu}^i \hat{S}^z \right) + D (\hat{S}^z)^2,$$

where $\hat{\mu}^\alpha$ and $\hat{S}^\alpha$ ($\alpha = x, y, z$) denote spatial components of spin-1/2 and spin-$S$ $(S \geq 1)$ operators, respectively. The parameter $J$ is the Heisenberg exchange interaction, $\Delta$ is the XXZ exchange anisotropy and $D$ is the uniaxial single-ion anisotropy, which affects higher-spin $S \geq 1$
only. The complete spectrum of the eigenvalues and eigenvectors of the Hamiltonian \([1]\) has been derived in our previous paper \([15]\), so we will list here for simplicity the final formulas for eigenenergies and eigenvectors only
\[
\varepsilon_{\pm(S + 1/2)} = \frac{S}{2} (J + 2DS) \rightarrow | \pm (S + 1/2) \rangle = |1/2, S\rangle,
\]
\[
e_{S}^z = \frac{1}{4} \left[ 1 \pm \sqrt{R_{S}^{2} + Q_{S}^{2}} \right],
\]
where \(S = \ldots, S\) and \(S_{z} = S^{z} + \mu \) is a corresponding energy level of negative eigenvalues \(\lambda\).

To study the bipartite entanglement we will use the concept of negativity \([16,13]\), which is defined in terms of negative eigenvalues \(\lambda_{i}\) of the partially transposed density matrix \(\rho^{T_{12}}\). The complete spectrum of the eigenvalues and the corresponding energy levels \(\varepsilon_{S}\) has been derived in our previous paper \([15]\), so we will list here for simplicity the final formulas for eigenenergies and eigenvectors only
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Figure 1: Density plots of the negativity in the plane \(D/J\) vs. \(\Delta\) for an integer (left panels) and half-odd-integer (right panels) spin \(S\), which correspond to different ground states \(|\pm S_{z}\rangle\).

3. Results and discussion

In the following, our discussion will be focused on the physically most interesting antiferromagnetic case \((J > 0)\), for which a great variety of ground states is expected. Fig. 1 illustrates the ground-state phase diagram in the \(D/J - \Delta\) plane commonly with the degree of entanglement exemplified through the respective zero-temperature density plot of the negativity. One immediately identifies that MSHDs with both half-odd-integer constituents (right panels) remain maximally entangled if the non-degenerate antiferromagnetic ground state \(|0\rangle\) is favoured. A non-degenerate character of a corresponding energy level \(e_{S}^z\) determines a simple structure of the negativity, \(N = c_{S}^{z}c_{S}^{-z}\), which results in the negativity \(N = 1/2\) completely independent of the strength of both assumed anisotropies. It is noteworthy that the degree of entanglement changes discontinuously at the relevant phase boundary of the \(|0\rangle\) ground state and then it continuously decreases with decreasing \(\Delta\) and/or \(D/J\). For half-odd-integer spins \(S\) and the specific exchange anisotropy \(\Delta\) one identifies \(S - 1/2\) phase boundaries, which merge together for a fully isotropic case \((\Delta = 1\) and \(D/J = 0\) as a consequence of energy equivalence between all \(|S_{z}\rangle\) ground states \(|\pm S_{z}\rangle\). On the other hand, the two-fold degeneracy of each \(|S_{z}\rangle\) ground state \(|\pm S_{z}\rangle\) for MSHDs with integer spins \(S\) (left panels) determines the different behaviour of the negativity in the most entangled ground state \(|\pm 1/2\rangle\).

Using definitions \([4,6]\) one obtains the relation
\[
N = \frac{1}{4} \left[ 1 - \frac{2D/J}{\sqrt{\alpha}} \right] \left[ \sqrt{5\sqrt{\alpha} + 3(1 - 2D/J) - 1} \right] ,
\]
where \(\alpha = (1 - 2D/J)^{2} + 4\Delta^{2}S(S + 1)\). It is clear that in the region of \(|\pm 1/2\rangle\) the degree of negativity strongly depends on the value of \(\Delta\), \(D/J\) and spin magnitude. Detailed numerical analysis (Fig. 2) exhibits existence of invariant negativity point at \(D/J = 1/2\) below which the negativity of dimer with a higher integer spin \(S\)
Figure 2: The dependence of a quantum negativity as a function of $D/J$ for different integer spin-$S$. Three exchange anisotropy limits are assumed. Open circles visualised in panel (b) denote the negativity at fully isotropic case, $\Delta = 1$ and $D/J=0$. The negativity at this point rapidly falls down with increasing spin value (open circles in Fig. 2(b)) of MSHD leads to the reduction of a degree of entanglement. The negativity smoothly decreases upon temperature rise. Similarly as in the previous case, the higher spin $S$ is responsible for a higher thermal stability and lower degree of bipartite entanglement. Nevertheless, the highest negativity in the fully isotropic case is significantly smaller in comparison to its anisotropic counterpart due to a degeneracy of the ground state discussed above; (iv) The reduction effect of an increasing spin magnitude $S$ on the degree of thermal entanglement is observed equally in case of $|\pm 1/2\rangle$ or $|0\rangle$ ground state if and only if $D/J < 1/2$ (Fig. 3(b)). In accordance to the zero-temperature analysis, the largest negativity of MSHDs with an arbitrary half-odd-integer spin $S$ is $N = 1/2$, whereas the negativity of MSHD with an integer spin $S$ saturates to a smaller value depending on both anisotropies; (iv) Stability as well as the degree of thermal entanglement of MSHD with $D/J > 1/2$ can be enhanced by increasing the spin size $S$. As illustrated in Fig. 4(d) the thermal entanglement can be additionally stabilized by half-odd-integer spins $S$, for which the low-temperature asymptotic limit of the negativity achieves the maximal possible value 1/2. The increasing degree of thermal entanglement driven by an increasing spin $S$ magnitude is also present in MSHDs with integer spin value $S$, however, the largest negativity does not exceed a half of the golden ratio $(\sqrt{5}-1)/4$.

Finally, let us look at the behaviour of a threshold temperature upon the variation of $D/J$ (Fig. 4). For a better lucidity the half-odd-integer spins $S$ are assumed only. As a result, the increasing spin value $S$ as well as the increasing $\Delta$ enlarges the threshold temperature between the entangled and separable state. It is evident that the single-ion anisotropy $D/J$ has an additional enhancing effect on the threshold temperature with a significant sharp minimum at a proximity of $D/J = 0$. While the threshold temperature for $D/J$ lying below the local minimum is a smooth continuous function, the threshold temperature for $D/J$ above the local minimum involves a few pronounced fluctuations, whose number increases as the spin magnitude $S$ increases. It is supposed that the origin of such different behaviour relates to the different ground-state spin arrangements, where the increasing temperature affecting the starting (almost) antiferromagnetic structure can temporarily favour one of other $|S^z\rangle$ ones, until the disentangled state is achieved.
Figure 3: Thermal behaviour of negativity for different spin $S$ in the mixed spin-(1/2, $S$) dimer for various $D/J$ anisotropy.

Figure 4: The behaviour of the threshold temperature of the model (1) for different spin $S$ and three values of $\Delta$.

determines the bipartite entanglement both, at zero as well as non-zero temperatures. The half-odd-integer character of both spins allows one to stabilize the maximally entangled antiferromagnetic ground state, for which the negativity is completely kept constant. On the other hand, the negativity of MSHDs with integer spins $S$ is not higher than $N = (\sqrt{5} - 1)/4$ and it can be tuned by magnetic anisotropies. Moreover, if $D/J > 1/2$, the negativity can be enhanced by increasing of the spin $S$ magnitudes though it does not reach the maximal value $N = 1/2$. In addition, the negativity in the fully isotropic MSHD ($\Delta = 1, D/J = 0$) is significantly smaller in comparison to its anisotropic counterpart as a consequence of $2S$-fold degeneracy. The increasing spin value $S$ rapidly reduces its maximal value from $N = 1/3$ achieved for the particular case with $S = 1$. In contradiction to the knowledge for $D/J = 0$, the increasing spin magnitude $S$ in region of $D/J > 1/2$ can be utilized to enhance not only the thermal stability but also the degree of thermal entanglement of MSHD. From the application point of view, MSHD with half-odd-integer spin $S$ is more favourable due to its saturation to a maximally entangled state. At the same time, the increasing spin $S$ additionally enlarges the threshold temperature between the entangled and disentangled state, which enhancement can be furthermore tuned by uniaxial single-ion anisotropy (of the easy-axis as well as the easy-plan type).

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