Thermal entanglement in an orthogonal dimer-plaquette chain with alternating Ising–Heisenberg coupling

H G Paulinelli, S M de Souza and Onofre Rojas

Departamento de Ciencias Exatas, Universidade Federal de Lavras, 37200-000, Lavras, MG, Brazil

Received 23 April 2013, in final form 12 June 2013
Published 3 July 2013
Online at stacks.iop.org/JPhysCM/25/306003

Abstract
In this paper we explore the entanglement in an orthogonal dimer-plaquette Ising–Heisenberg chain, assembled between plaquette edges, also known as orthogonal dimer plaquettes. The quantum entanglement properties involving an infinite chain structure are quite important, not only because the mathematical calculation is cumbersome but also because real materials are well represented by infinite chains. Using the local gauge symmetry of this model, we are able to map onto a simple spin-1 like Ising and spin-1/2 Heisenberg dimer model with single effective ion anisotropy. Thereafter this model can be solved using the decoration transformation and transfer matrix approach. First, we discuss the phase diagram at zero temperature of this model, where we find five ground states, one ferromagnetic, one antiferromagnetic, one triplet–triplet disordered and one triplet–singlet disordered phase, beside a dimer ferromagnetic–antiferromagnetic phase. In addition, we discuss the thermodynamic properties such as entropy, where we display the residual entropy. Furthermore, using the nearest site correlation function it is possible also to analyze the pairwise thermal entanglement for both orthogonal dimers. Additionally, we discuss the threshold temperature of the entangled region as a function of Hamiltonian parameters. We find a quite interesting thin reentrance threshold temperature for one of the dimers, and we also discuss the differences and similarities for both dimers.

1. Introduction

Recently, several theoretical investigations have been dedicated to quantum entanglement, which is one of the most fascinating types of correlations that can be shared only among quantum systems [1]. In recent years, much effort has been devoted to characterizing qualitatively and quantitatively the entanglement properties of condensed matter systems, which are the natural candidates for application in quantum communication and quantum information. In this sense, it is quite relevant to study the entanglement of solid state systems such as spin chains [2]. The Heisenberg chain is one of the simplest quantum systems that exhibits entanglement, due to the Heisenberg interaction being nonlocalized in the spin system. Several studies have been made on the threshold temperature for pairwise thermal entanglement in the Heisenberg model with a finite number of qubits. Thermal entanglement of the isotropic Heisenberg chain has been studied in the absence [3] and in the presence of an external magnetic field [4].

On the other hand, quasi-two-dimensional magnets have attracted interest since the 1990s, such as the quasi-two-dimensional magnet CaV$_4$O$_9$ [5], which has a layered structure where the magnetic V$^{4+}$ ions have spin 1/2 and form a 1/5-depleted square lattice. In addition to polycrystalline SrCu$_2$(BO$_3$)$_2$ having a two-dimensional (2D) orthogonal network of Cu dimers, this cuprate provides a 2D spin-gap system in which the ground state can be solved exactly [6, 7]. These quasi-two-dimensional systems are topologically equivalent to the theoretical model proposed by Shastry and Sutherland [8].
Motivated by the above real materials, Ivanov and Richter [9] proposed the class of one-dimensional Heisenberg spin models (plaquette chains) related to the real materials [5–7], for which the zero temperature magnetic properties were analyzed through numerical and analytical results [9, 10]. Meanwhile, in [11] the sequence of first-order quantum phase transitions in a frustrated spin half dimer-plaquette chain was discussed. A detailed investigation of the first-order quantum phase transition of the orthogonal dimer spin chain was also made by Koga et al [12], as well as the frustration-induced phase transitions in the spin-3 orthogonal dimer chain [13].

A more recent investigation was made by Ohanyan and Honecker [14], where they discussed the magnetothermal properties of the Ising–Heisenberg orthogonal dimer chain with triangular XXZ clusters. Furthermore, in the last decade several quasi-one-dimensional Ising–Heisenberg models such as the diamond chain have been intensively investigated, mainly with respect to the thermodynamic properties and geometric frustration [15–18], the magneto-caloric effect [19], as well as the thermal entanglement [20, 21], among other physical quantities. Some other variants of the Ising–Heisenberg model have also been considered, such as the Ising–Hubbard model [22] and the Hubbard model in the quasi-atomic limit [23] besides spinless electrons [24] in the diamond chain.

The outline of this work is as follows. In section 2 we present the dimer-plaquette Ising–Heisenberg chain; the zero temperature phase diagram is also discussed. In section 3 we present the dimer-plaquette Ising–Heisenberg chain model whose Hamiltonian is given by

\[ H = -J_0[\sigma_{a,i}^z + \sigma_{b,i}^z + (\sigma_{a,i+1}^z + \sigma_{b,i+1}^z)\sigma_{d,i}^z], \]

(1)

with \( J'(\sigma_{a,i}, \sigma_{b,i}) = \sigma_{a,i}^z \sigma_{b,i}^z + \sigma_{a,i}^y \sigma_{b,i}^y + \Delta \sigma_{a,i}^z \sigma_{b,i}^z, \)

(2)

where \( \sigma_{\gamma,i}^\alpha \) are the spin operators, also known as Pauli matrices (with \( \alpha = \{x, y, z\} \)), at plaquette \( i \) for particles \( \gamma = \{a, b, c, d\} \); for details see figure 1. The thick line corresponds to Heisenberg coupling, while the thin line corresponds to Ising coupling. The Ising coupling parameter is denoted by \( J_0 \), whereas \( J (J') \) represents the \( x \) and \( y \) components of the Heisenberg coupling, and by \( \Delta (\Delta') \) we mean the anisotropic \( (z\text{-component}) \) coupling in the Heisenberg term for the \( ab\)-dimer and \( cd\)-dimer respectively.

To transform this model into the well known mixed spin ‘Ising’–Heisenberg model, we use the following definition: \( S_i^j = \sigma_{a,i}^z + \sigma_{b,i}^z \). By the use of the \( S_i^j \) definition we obtain the identity \( (S_i^j)^2 = 2 + 2\sigma_{a,i}^x \sigma_{b,i}^x \). Thereafter, we can easily establish the following transformation:

\[ J'(\sigma_{a,i}, \sigma_{b,i})_i = \frac{J'}{2} \frac{\Delta' - J'}{2} (S_i^j)^2 = -2J' + \Delta', \]

(3)

and by \( S_i^2 \) we just denote \( S_i^2 = S_i \cdot S_i \); therefore this matrix is given by

\[ S_i^2 = 4 \begin{pmatrix} 2 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 2 \end{pmatrix}. \]

(4)

Rewriting the Hamiltonian in terms of operators \( S_i^j \) and \( S_i^2 \) we have an Ising–Heisenberg chain model whose Hamiltonian is given by \( H = H_0 + H' \), with \( H_0 = (2J' + \Delta')N \). Therefore, the transformed Hamiltonian reduces to

\[ H' = -\sum_{i=1}^N \left\{ \frac{J'}{4} (S_i^2 + S_{i+1}^2) + \frac{\Delta' - J'}{4} (S_i^2)^2 + (S_{i+1}^2)^2 \right\} + J_0 (S_i^c \sigma_{a,i}^z + \sigma_{d,i}^z S_{i+1}^c), \]

(5)

We can observe from equation (4) that the matrix is a \( 2 \times 2 \) block matrix; hence, we can diagonalize this block matrix. It is interesting to note that the matrix \( S_i^c \) is still diagonal in the new basis, due to the corresponding \( 2 \times 2 \) block matrix being null. Then, this means that we can simultaneously diagonalize both matrices \( S_i^c \) and \( S_i^2 \). Recall that \( S_i^c \) and \( S_i^2 \) are commutative.
operators. Therefore, the diagonal matrices are expressed by

$$S_i^\pm = \begin{bmatrix} 8 & 0 & 0 & 0 \\ 0 & 8 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 8 \end{bmatrix} \quad \text{and} \quad S_i^\mp = \begin{bmatrix} 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -2 \end{bmatrix},$$

and their corresponding eigenvector states are expressed as

$$|\tau_{+1}\rangle = |+\rangle, \quad (7)$$

$$|\tau_0\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} + \\ - \\ + \\ - \end{bmatrix}, \quad (8)$$

$$|\tau_{-1}\rangle = |-\rangle, \quad (9)$$

$$|\tau_{-1}\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} + \\ - \\ - \\ + \end{bmatrix}. \quad (10)$$

The effective Ising ‘spin’ in Hamiltonian (5) can be understood as a composition of one triplet state and one singlet state.

This transformation is possible because the local gauge symmetry is only satisfied by Hamiltonian (1) when the Ising couplings $ac (ad)$ and $bc (bd)$ are identical.

### 2.1. The zero temperature phase diagram

In order to analyze the phase diagram of the orthogonal dimer plaquette, we assume the particular case $J' = J$ and $\Delta' = \Delta$, following the parameters used in the literature [11–13].

The dimer-plaquette Ising–Heisenberg chain described by the Hamiltonian equation (1) exhibits five ground states. These states are expressed as

$$|\text{FM}\rangle = \prod_{i=1}^{N} |+\rangle_i \otimes |+\rangle_i, \quad (11)$$

$$|\text{AFM}\rangle = \prod_{i=1}^{N} |+\rangle_i \otimes |-\rangle_i. \quad (12)$$

For the ferromagnetic (FM) phase and the antiferromagnetic (AFM) phase the corresponding eigenvalues are given by

$$E_{\text{FM}} = -2J' - 2\Delta' - \Delta - 4J_0,$$

$$E_{\text{AFM}} = -2J' - 2\Delta' - \Delta + 4J_0.$$  

The other phase are composed of dimers in triplet–triplet (TT) phase and triplet–singlet (TS) phase,

$$|\text{TT}\rangle = \prod_{i=1}^{N} |\tau_0\rangle_i \otimes \frac{1}{\sqrt{2}}(|+\rangle_i + |-\rangle_i), \quad (13)$$

$$|\text{TS}\rangle = \prod_{i=1}^{N} |\tau_0\rangle_i \otimes \frac{1}{\sqrt{2}}(|+\rangle_i - |-\rangle_i). \quad (14)$$

Figure 2. (a) Phase diagram at zero temperature as the dependence of $J$ and $\Delta$ for a fixed value of $J_0 = 1$. (b) Phase diagram at zero temperature as the dependence of $J_0$ and $\Delta$ for a fixed value of $J = 1$.

where the corresponding eigenvalues become

$$E_{\text{TT}} = \Delta - 2J - 4J', \quad E_{\text{TS}} = \Delta + 2J.$$

It is worth mentioning that the state given by equations (13) and (14) becomes a frustrated state only when $J = 0$ (Ising limit).

Finally, the dimer–antiferromagnetic (DFA) state can be expressed by

$$|\text{DFA}\rangle = \prod_{i=1}^{N/2} |+\rangle_i \otimes |\eta_{2,-2}\rangle_i \otimes |-\rangle_i \otimes |\eta_{2,-2}\rangle_i, \quad (15)$$

with

$$|\eta_{2,-2}\rangle = \left( |+\rangle_i + \vartheta |+\rangle_i \right) / \sqrt{1 + \vartheta^2}, \quad (16)$$

and

$$\vartheta = \frac{\sqrt{4J_0^2 + J^2} + 2J_0}{J}. \quad (17)$$

Hereafter the corresponding dimer–antiferromagnetic eigenvalue becomes

$$E_{\text{DFA}} = -2J' - 2\Delta' + \Delta - 2\sqrt{4J_0^2 + J^2}.$$  

In order to display the phase diagram at zero temperature, we plot $J$ versus $\Delta$, assuming a fixed value of $J_0 = 1$ (−1) for FM (AFM) respectively. As shown in figure 2(a), for $\Delta < -2$, there is a boundary between the TS and TT states at $J = 0$, whereas for $-2 \leq \Delta \leq 0.5$ the state TT (TT) is limited by the DFA region whose boundary is given by $\Delta = 2|J| - \sqrt{4 + J^2}$, when $J > 0 (J < 0)$ respectively. Meanwhile, for $\Delta \geq 0.5$ the state TS (TT) is limited by the FM (AFM) region $\Delta = |J| - 1$. Furthermore, the boundary between the DFA and FM (AFM) regions is represented by the curve $\Delta = \sqrt{4 + J^2} - 2$.

Meanwhile, in figure 2(b), we observe the phase diagram from another viewpoint, $\Delta$ against $J_0$, assuming fixed $J = 1$. In this picture the TS and TT phases are displayed in the same region, while the AFM and FM states are illustrated for $J_0 > 0 (J_0 < 0)$ respectively. The boundary between FM (AFM) and TT (TS) is given by $\Delta = 1 - |J_0|$ when $|J_0| < 2/3$, whereas the DFA region appears when $|J_0| > 2/3$, which is limited by the TT (TS) region, and this boundary curve becomes
\[ \Delta = 2 - \sqrt{4J_0^2 + 1}; \text{ finally the boundary between the FM and AFM regions is described by the curve } \Delta = \sqrt{4J_0^2 + 1 - 2|J_0|}. \]

3. The thermodynamics of the model

The method used will be the decoration transformation proposed in the early 1950s by Syozı [25] and Fisher [26]. Afterward this approach was the subject of study in [27], for the case of multi-spins. A similar generalization was developed by Strečka [28] for a hybrid system (e.g. Ising–Heisenberg). Another interesting variant of this transformation was proposed in [29], where a direct transformation was proposed instead of several step by step transformations. Consequently, the decoration transformation approach was also discussed previously in [29], where a direct transformation could be applied to electron coupling systems; this has been applied for the case of spinless fermions on the diamond structure [24], and as well as for the Hubbard model in the quasi-atomic limit [23].

In order to study the thermodynamics of the dimer-plaque Ising–Heisenberg chain we will use the decoration transformation proposed in [29] together with the usual transfer matrix technique [30]. Therefore, let us start by considering the partition function as follows:

\[ Z_N = e^{-\beta H_0} \text{tr} \left( \prod_{i=1}^{N} e^{-\beta H'} \right), \quad (18) \]

where \( \beta = 1/\kappa T \), with \( k \) being the Boltzmann constant and \( T \) the absolute temperature, and assuming \( H' \) is given by equation (5).

The effective model can be solved by the usual transfer matrix approach [30], inasmuch as the transfer matrix of the Hamiltonian (5) is reduced to

\[ T = \begin{bmatrix}
    w_{1,1} & w_{1,0}x^2 & w_{1,0} & w_{1,-1} \\
    w_{1,0}x^2 & w_{0,0}x^4 & w_{0,0}x^2 & w_{1,0}x^2 \\
    w_{1,0} & w_{0,0}x^2 & w_{0,0} & w_{1,0} \\
    w_{1,-1} & w_{1,0}x^2 & w_{1,0} & w_{1,1}
\end{bmatrix}, \quad (19) \]

with

\[ w_{1,1} = x^2z^2[1 + x^2 + \lambda(1 + x^2)], \quad (20) \]
\[ w_{1,0} = x^2z^2[1 + x^2 + \lambda(1 + x^2)], \quad (21) \]
\[ w_{1,-1} = x^2z^2[1 + x^2 + \lambda(1 + x^2)], \quad (22) \]
\[ w_{0,0} = 2z + \lambda x^2. \quad (23) \]

where we have introduced the following notations: \( x = e^{\beta J}, \quad z = e^{\beta \Delta}, \quad \lambda = e^{\beta J}, \quad \lambda' = e^{\beta \Delta'}, \quad \lambda'' = e^{\beta J_0} \). Furthermore, we define also the following exponentials: \( x_1 = e^{\beta J^2 + J_0} / z^2 \) and \( x_2 = e^{\beta J_2 + J_0} \).

In order to diagonalize the transfer matrix \( T \), we perform the determinant of the transfer matrix, which is expressed as follows:

\[ \lambda(\lambda^2 - a_1 \lambda + a_0)(\lambda - w_{1,1} + w_{1,-1}) = 0. \quad (24) \]

Here, the coefficients of the quadratic term equation (24) are given by

\[ a_1 = w_{1,1} + w_{0,0}(1 + x^4) + w_{1,-1}, \quad (25) \]
\[ a_0 = (1 + x^4)[w_{0,0}(w_{1,1} + w_{1,-1}) - 2w_{1,0}']. \]

Therefore, the eigenvalues can be expressed as

\[ \lambda_0 = \frac{1}{2} \left( a_1 + \sqrt{a_1^2 - 4a_0} \right), \quad (26) \]
\[ \lambda_1 = \frac{1}{2} \left( a_1 - \sqrt{a_1^2 - 4a_0} \right), \quad (27) \]
\[ \lambda_2 = x^2z^2 \left( 1 + \frac{(x^2 + x^2 - x_2 - x_2^2)}{z} \right). \quad (28) \]

In the thermodynamic limit, the free energy per unit cell is given by only the largest eigenvalue of the transfer matrix, and for our case we can easily verify that the first eigenvalue \( \lambda_0 \) always becomes the largest one. Thus, the free energy can be expressed by the following relation:

\[ f = 2J' + \Delta' - \frac{1}{\beta} \ln(\lambda_0). \quad (30) \]

The first term of the free energy is a trivial constant energy, obtained during the local gauge transformation, which is irrelevant for thermodynamic quantities. Note that the free energy is valid for arbitrary values of \( J' \) and \( \Delta' \), although here we consider only a particular case \( J' = J \) and \( \Delta' = \Delta \), following the parameters used in the literature [11–13]. Therefore, any additional properties can be obtained straightforwardly from equation (30).

3.1. Entropy and specific heat

In order to proceed with our discussion concerning the thermodynamic properties, let us illustrate the entropy \( (S = -\beta f/\partial T) \) in figure 3(a) for the low temperature limit as a function of \( \Delta \) and \( J \), whereas in figure 3(b) the entropy is illustrated as a function of \( \Delta \) and \( J_0 \). The dark region corresponds to higher entropy, while the white region corresponds to zero entropy. However, as soon as the temperature decreases the entropy goes to zero, except, for \( J = 0 \) and \( \Delta \leq -2 \) (pure Ising chain), the dark line will remain when the temperature decreases, leading to a residual entropy \( S_0 = 2 \ln(2) \), which illustrates the geometric frustration region of the orthogonal plaque Ising chain.

Finally, we also discuss another interesting thermodynamic quantity called the specific heat \( (C = -T \beta^2 f/\partial T^2) \). In figure 4, we plot the specific heat as a function of the temperature \( T \) for a fixed coupling parameter \( J_0 = 1.0 \) and a fixed value of \( J = 1.0 \). By a solid line we represent the specific heat curve when \( \Delta = 0, 0.5 \) and 1.0, while, by a dashed line we illustrate the specific heat for \( \Delta = -0.5 \) and \( -1.0 \). For the anisotropic parameter values \( \Delta = \pm 0.5 \) and 0, the plot illustrates a small anomalous peak due to
the zero temperature phase transition influence, although for Δ = ±1.0 this anomalous peak disappears, because there is no zero temperature phase transition in the neighborhood.

3.2. Pair correlation function

The nearest site correlation function between dimers can be obtained using a derivative of the free energy given by equation (30). Then, in order to perform the derivative of free energy, we need to assume the parameters J′ and J as independent parameters; similarly Δ′ and Δ are also considered as independent parameters. Although for physical quantities the term 2J′ + Δ′ in the free energy is irrelevant, this term cannot be neglected when we calculate the correlation function as expressed below:

\[
\langle \sigma_i^z \sigma_j^z \rangle = \frac{1}{2} \frac{\partial f}{\partial J} = -1 + \frac{J}{\Delta} \frac{\partial \lambda_0}{\partial \lambda_0} \frac{\partial \lambda_0}{\partial \lambda_0},
\]

\[
\langle \sigma_i^x \sigma_j^z \rangle = -\frac{\partial f}{\partial \Delta} = -1 + \frac{J}{\Delta} \frac{\partial \lambda_0}{\partial \lambda_0} \frac{\partial \lambda_0}{\partial \lambda_0},
\]

\[
\langle \sigma_i^y \sigma_j^z \rangle = -\frac{\partial f}{\partial J} = \frac{J}{\Delta} \frac{\partial \lambda_0}{\partial \lambda_0} \frac{\partial \lambda_0}{\partial \lambda_0},
\]

\[
\langle \sigma_i^z \sigma_j^y \rangle = -\frac{\partial f}{\partial J} = \frac{J}{\Delta} \frac{\partial \lambda_0}{\partial \lambda_0} \frac{\partial \lambda_0}{\partial \lambda_0}.
\]

Here, we present the relation of the correlation function in terms of the largest eigenvalue of the transfer matrix λ0.

In order to accomplish our analysis concerning the correlation function we display in figure 5 the correlation function given by equations (31)–(34), as a function of temperature, assuming conveniently fixed parameters J0 = 1.0 and J = 1.0 close to the phase transition illustrated in figure 2. Thus, figure 5(a) is for the case of an anisotropic parameter Δ = −0.3, and we observe how the correlation function at low temperature behaves quite similarly for both the ab-dimer and the cd-dimer; for example the z-component of the pair correlation is negative because the ground state energy is TT (TS), while the xy-component is positive. However, as soon as the temperature increases the difference becomes relevant. It is worth emphasizing that the correlation function ⟨σ_i^z σ_j^z⟩ turns positive at finite temperature T ≈ 0.7 and for higher temperature once again the correlation function becomes negative at a temperature of around T ≈ 2.5, becoming a small negative amount. Similarly, figure 5(b) is for an anisotropic parameter Δ = 0.3. The ab-dimer and cd-dimer behave quite similarly in the low temperature limit; the z-component of the pair correlation is positive because it corresponds to the FM (AFM) region, in agreement with equations (11) and (12), while the xy-component correlation function is zero. Nevertheless, for higher temperature this difference is significant: the ⟨σ_i^z σ_j^z⟩ and ⟨σ_i^z σ_j^z⟩ have a maximum at finite temperature, while the ⟨σ_i^z σ_j^z⟩ is a monotonic decreasing function and ⟨σ_i^z σ_j^z⟩ decreases faster, becoming negative at T ≈ 0.9; for higher temperature at around T ≈ 2.4 the ⟨σ_i^z σ_j^z⟩ correlation function becomes a positive quantity.
4. Thermal entanglement

Another interesting property we consider in this work is the quantum entanglement of the Ising–Heisenberg orthogonal dimer-plaquette model. As a measure of entanglement for two arbitrary mixed states of dimers, we use the quantity called concurrence [31], which is defined in terms of the reduced density matrix $\rho$:

$$C(\rho) = \max\{0, 2\Lambda_{\max} - \text{tr}\sqrt{R}\},$$

(35)

assuming

$$R = \rho \sigma^y \otimes \sigma^y \sigma^y \otimes \sigma^y,$$

(36)

where $\Lambda_{\max}$ is the largest eigenvalue of the matrix $\sqrt{R}$ and $\rho^*$ represents the complex conjugate of the matrix $\rho$, with $\sigma^y$ being the Pauli matrix.

For the case of an infinite chain, the reduced density operator elements [32] can be expressed in terms of the correlation function between two entangled particles [33]; consequently the concurrence for the ab-dimer becomes

$$C_{ab} = \max\{0, |\langle \sigma^x_a \sigma^x_b \rangle | - \frac{1}{2} |1 + \langle \sigma^z_a \sigma^z_b \rangle|\}.$$  

(37)

Similarly the concurrence for the cd-dimer reads

$$C_{cd} = \max\{0, |\langle \sigma^x_c \sigma^x_d \rangle | - \frac{1}{2} |1 + \langle \sigma^z_c \sigma^z_d \rangle|\}.$$  

(38)

Surely, we can also obtain an equivalent result using the approach described in [20].

It is worth mentioning that the zero temperature entanglement for the $ab$-dimer is maximally entangled in the TS and TT regions, $C_{ab} = 1$, while in all other regions the $ab$-dimer becomes untangled ($C_{ab} = 0$). Meanwhile, the $cd$-dimer is also maximally entangled in the same (TS and TT) regions, $C_{cd} = 1$; additionally the DFA region now also becomes an entangled region whose concurrence is given by $C_{cd} = \frac{|J|}{|J|^2 + J^2}$ and it depends on $J$ and $J_0$. It is worth noticing that when $J = 0$ this region becomes untangled, which is perfectly coherent since the model reduces to an orthogonal plaquette Ising chain. Another special possibility is when $J_0 = 0$; the orthogonal dimer plaquette reduces simply to independent entangled dimers, while the FM and AFM regions are untangled, $C_{cd} = 0$.

In figure 6 the concurrence $C$ is plotted as a function of the temperature: for $\Delta = -1$ the dashed and solid lines correspond to the $ab$-dimer and $cd$-dimer respectively. However, the $ab$-dimer entanglement vanishes for $T \approx 2.9$, while for the $cd$-dimer the entanglement vanishes at $T \approx 4.0$. For weaker anisotropic coupling ($\Delta$) this difference becomes more significant. For example, for $\Delta = -0.24$, for the $cd$-dimer (solid line) the entanglement vanishes for $T \approx 2.25$, whilst for the $ab$-dimer the entanglement vanishes at $T \approx 0.28$ (dashed line). For a slightly weaker anisotropic parameter $\Delta = -0.22$, the $ab$-dimer becomes untangled for any temperature, while for the $cd$-dimer the entanglement vanishes at $T \approx 2.24$.

4.1. Threshold temperature

The threshold temperature can be obtained when the $ab$-dimer concurrence becomes null ($|\langle \sigma^x_a \sigma^x_b \rangle | = \frac{1}{2} |1 + \langle \sigma^z_a \sigma^z_b \rangle|)$, and similarly for the $cd$-dimer, the concurrence will become null when $|\langle \sigma^x_c \sigma^x_d \rangle | = \frac{1}{2} |1 + \langle \sigma^z_c \sigma^z_d \rangle|$.

The threshold temperature is illustrated in figure 7 as a function of the anisotropic parameter for fixed values of $J_0 = 1$ and $J = 1$. The dashed line corresponds to the $ab$-dimer threshold temperature, and in the low temperature limit, the threshold temperature leads to $T_{th} = 2 - \sqrt{3}$. The solid line represents the $cd$-dimer threshold temperature; in the low temperature limit it leads to $T_{th} = \sqrt{3} - 2$. It is worth highlighting that the threshold temperature for the $cd$-dimer exhibits a thin reentrance around $\Delta = 0.1$. 

![Figure 6](image6.png)

**Figure 6.** Concurrence for several values of the anisotropic parameter as a function of $T$, assuming fixed $J_0 = 1$ and $J = 1$. The dashed line corresponds to the $ab$-dimer while the solid line represents the $cd$-dimer.

![Figure 7](image7.png)

**Figure 7.** Threshold temperature $T_{th}$ as a function of $\Delta$, for fixed $J_0 = 1$ and $J = 1$. The dashed line corresponds to the $ab$-dimer, while the solid line represents the $cd$-dimer.
Another way to display the entanglement phase diagram is in units of the threshold temperature, as displayed in figure 8; the boundary between the entangled region and the untangled region is given by a solid (red) line. The black region corresponds to the maximally entangled region, while the light gray region corresponds to weak concurrence, and similarly dark gray corresponds to strong concurrence. The entangled phase diagram of \( J \) against \( \Delta \) in units of \( T_{th} \) behaves quite similar for both the \( ab \)-dimer and the \( cd \)-dimer, although for the \( ab \)-dimer the entangled region becomes relevant only for \( \Delta \geq -3 \) and small values of \( J \), while for the \( cd \)-dimer the untangled region becomes relevant only for \( \Delta \geq -1 \) and small values of \( J \). Certainly this is in agreement with the zero temperature phase diagram displayed in figure 2(a).

An additional density plot of the entangled phase diagram is displayed in figure 9 in terms of \( \Delta \) and \( J_0 \), once again in units of \( T_{th} \); the phase diagram for the \( ab \)-dimer is given in figure 2(a), and the phase diagram for the \( cd \)-dimer is illustrated in figure 2(b). Here, we observe that the phase diagrams of the \( ab \)-dimer and the \( cd \)-dimer are quite different, but are still closely related to the zero temperature phase diagram illustrated in figure 2(b). However, the darkest (strongly entangled) regions are very similar for both dimers.

5. Conclusion

In this work, we studied the dimer-plaquette Ising–Heisenberg chain, assembled between plaquette edges, also known as orthogonal dimer plaquettes [9–14]. Using the local gauge symmetry of this model, we were able to map onto a simple spin-1 like Ising and spin-1/2 Heisenberg dimer model with single effective ion anisotropy. Thereafter, this model could be solved using the decoration transformation [25–27, 29] and transfer matrix approach. First, we discussed the phase diagram at zero temperature of this model, where we found five ground states, as illustrated in figure 2, one ferromagnetic, one antiferromagnetic, one triplet–triplet disordered and one triplet–singlet disordered phase, beside a dimer ferromagnetic–antiferromagnetic phase. It is interesting to remark that, in the limit of the pure Ising model, this exhibits a frustrated region. Furthermore, the thermodynamic properties were discussed, such as the entropy and the specific heat as well as the correlation function. Additionally, using the nearest site correlation function it was possible to analyze the pairwise thermal entanglement for both the \( ab \)-dimer and the \( cd \)-dimer. Moreover, the threshold temperature of the entangled region was discussed as a function of the Hamiltonian parameters. There are some significant differences between the two dimers (\( ab \)-dimers and \( cd \)-dimers); this is in agreement in the low temperature limit. However, for strong entanglement, both dimers are quite similar. As a consequence of this difference, we were able to illustrate one interesting result, regarding the reentrance type of the threshold temperature for the \( cd \)-dimer, although for the \( ab \)-dimer there is no reentrance temperature.

Acknowledgments

HGP thanks CAPES for full financial support, while SMS and OR thank FAPEMIG and CNPq for partial financial support. OR also thanks ICTP for partial financial support.

References

[1] Gühne O and Tóth G 2009 Phys. Rep. 474 1
[2] O’Connor K M and Wootters W K 2001 Phys. Rev. A 63 052302
[3] Wang X 2002 Phys. Rev. A 66 044305
[4] Arnesen M C, Bose S and Vedral V 2001 Phys. Rev. Lett. 87 017901
[5] Taniguchi S et al 1995 J. Phys. Soc. Japan 64 2758
[6] Miyahara S and Ueda K 1999 Phys. Rev. Lett. 82 3701
[7] Kageyama H et al 1999 Phys. Rev. Lett. 82 3168
[8] Shastry B S and Sutherland B 1981 Physica 108B 1069
[9] Ivanov N B and Richter J 1997 Phys. Lett. A 232 308
[10] Richter J, Ivanov N B and Schulenburg J 1998 J. Phys.: Condens. Matter 10 3635
[11] Schulenburg J and Richter J 2002 Phys. Rev. B 65 054420
[12] Koga A, Okunishi K and Kawakami N 2000 Phys. Rev. B 62 5558
[13] Koga A and Kawakami N 2002 Phys. Rev. B 65 214415
[14] Ohanyan V and Honecker A 2012 Phys. Rev. B 86 054412
[15] Rojas O, de Souza S M, Ohanyan V and Khurshudyan M 2011 Phys. Rev. B 83 094430
[16] Valverde J S, Rojas O and de Souza S M 2008 J. Phys.: Condens. Matter 20 345208
[17] Canova L, Strečka J and Jascur M 2006 J. Phys.: Condens. Matter 18 4967
[18] Canova L, Strecka J and Lucivjansky T 2009 Condens. Matter Phys. 12 353
[19] Pereira M S S, de Moura F A B F and Lyra M L 2009 Phys. Rev. B 79 054427
[20] Rojas O, Rojas M, Ananikian N S and deSouza S M 2012 Phys. Rev. A 86 042330
[21] Ananikian N S, Ananikyan L N, Chakhmakhchyan L A and Rojas O 2012 J. Phys.: Condens. Matter 24 256001
[22] Lisnii B M 2011 Low Temp. Phys. 37 296
[23] Rojas O, de Souza S M and Ananikian N S 2012 Phys. Rev. E 85 061123
[24] Rojas O and de Souza S M 2011 Phys. Lett. A 375 1295
[25] Syozi I 1951 Prog. Theor. Phys. 6 341
[26] Fisher M 1959 Phys. Rev. 113 969
[27] Rojas O, Valverde J S and de Souza S M 2009 Physica A 388 1419
[28] Strečka J 2010 Phys. Lett. A. 374 3718
[29] Rojas O and de Souza S M 2011 J. Phys. A: Math. Theor. 44 245001
[30] Baxter R J 1982 Exactly Solved Models in Statistical Mechanics (New York: Academic)
[31] Wootters W K 1998 Phys. Rev. Lett. 80 2245
[32] Bukman D J, An G and van Leeuwen J M J 1991 Phys. Rev. B 43 13352
[33] Amico L, Osterloh A, Plastina F and Fazio R 2004 Phys. Rev. A 69 022304