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Persistence of entanglement in thermal states of spin systems

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Abstract

We study and compare the persistence of bipartite entanglement (BE) and multipartite entanglement (ME) in one-dimensional and two-dimensional spin XY models in an external transverse magnetic field under the effect of thermal excitations. We compare the threshold temperature at which the entanglement vanishes in both types of entanglement. We use the entanglement of formation as a measure of the BE and the geometric measure to evaluate the ME of the system. We have found that in both dimensions in the anisotropic and partially anisotropic spin systems at zero temperatures, all types of entanglement decay as the magnetic field increases but are sustained with very small magnitudes at high field values. Also we found that for the same systems, the threshold temperatures of the nearest neighbour (nn) BEs are higher than both of the next-to-nearest neighbour BEs and MEs and the three of them increase monotonically with the magnetic field strength. Thus, as the temperature increases, the ME and the far parts BE of the system become more fragile to thermal excitations compared to the nn BE. For the isotropic system, all types of entanglement and threshold temperatures vanish at the same exact small value of the magnetic field. We emphasise the major role played by both the properties of the ground state of the system and the energy gap in controlling the characteristics of the entanglement and threshold temperatures. In addition, we have shown how an inserted magnetic impurity can be used to preserve all types of entanglement and enhance their threshold temperatures. Furthermore, we found that the quantum effects in the spin systems can be maintained at high temperatures, as the different types of entanglements in the spin lattices are sustained at high temperatures by applying sufficiently high magnetic fields.

(Some figures may appear in colour only in the online journal)

1. Introduction

The state of a classical composite system is described in the phase space as a product of its individual constituents' separate states, whereas the state of a composite quantum system is expressed in the Hilbert space as a superposition of tensor products of its individual subsystems' states. Therefore, the state of a quantum composite system is not necessarily expressible as a product of the individual quantum subsystems' states. This peculiar property of quantum systems is called entanglement, which has no classical analogue [1]. Recently, the interest in studying quantum entanglement was sparked by the development in the fields of quantum information and quantum computing, which was initiated in the 1980s by the pioneering work of Benioff, Bennett, Deutsch, Feynman and Landauer [2–8]. Although there is still no complete theory that can quantify the entanglement of a general multipartite system in a pure or mixed state, there are few cases where we have successful entanglement measures. Most importantly, bipartite systems in a pure state and mixed state of two spin-1/2 possess such measures, also the pure and mixed multipartite systems using geometric measures, such as geometric entanglement

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(GE) and relative entanglement [9–14]. Quantum information processing and quantum computations can only be performed in a many-body system with very complicated arrangements concerning the properties of that system [15]. The building unit, smallest for storing information in such a system (qubit), has to be a well defined two state quantum entity that can be easily addressed, manipulated and readout. The basic idea is to define a certain quantum degree of freedom to serve as a qubit, such as the charge, orbital or spin angular momentum. The next step is to define a controllable mechanism to form the coupling between two individual qubits in such a way as to produce a fundamental quantum computing gate. Furthermore, we have to be able to coherently manipulate such a mechanism to provide an efficient computational process. On the other hand, quantum phase transitions in many-body systems are accompanied by a significant change in the quantum correlations within the system, which led to a great interest in investigating the behaviour of quantum entanglement close to the critical points of transitions [16–19].

All these facts and developments sparked great interest in studying entanglement properties in many-body systems in general and particularly in quantum spin systems in the presence of external magnetic fields at zero and finite temperatures [20, 21]. There has been special focus on studying entanglement in one-dimensional (1D) spin chains, utilizing the possession of exact analytic solutions for many of these systems [17, 19, 22–26]. The raised question of the multipartite entanglement (ME) versus bipartite entanglement (BE) and whether they have to coexist and which one is the actual resource for the critical behaviour in many-body systems has stimulated many investigations. To address this problem, several works have focused on comparing ME with BE in quantum spin systems. Some of these works made use of the one tangle [27, 28] as well as the concurrence [29] for that purpose without explicitly evaluating the global entanglement in the system. The one tangle τ_1 represents the entanglement between a single spin with the rest of the system at zero temperature, which is equal to $4\,det\,\rho^{(1)}$, where $\rho^{(1)}$ is the single site reduced density matrix. On the other hand, the sum of the squared of pairwise concurrences, $\sum_{i\neq j} C^2_{i,j}$, defines another quantity τ_2 representing the weight of the pairwise entanglements in the system. The ratio $R = \tau_2/\tau_1$ was introduced as a measure of the fraction of the total entanglement attributed to the pairwise correlations.

The quantification of the global ME in a many-body system is a very hard task as it usually requires the solution of a big set of variational equations and the difficulty of the problem increases nonlinearly with the dimension of the Hilbert space. Few different measures of global entanglement have been proposed, the most common among them are the relative entropy of entanglement [13, 30], the robustness of entanglement [31], polynomial measure [32] and the geometric measure [14]. Particularly, the geometric measure determines the distance between the state under consideration and the closest product state in the Hilbert space. This measure has been used intensively to study the ME in many-body systems and especially the 1D spin chain systems utilizing the exact solutions that these systems have [18, 33–38].

Natural systems of interest have strong interaction with their environment, which causes decoherence effects [39, 40]. Particularly, practical many-body systems are required to function at finite temperatures, which means that the system will be exposed to thermal excitations and therefore its mixed thermal states should be fully studied and understood. Evaluating the density matrix of mixed thermal states of many-body systems is a very hard task due to the large size of the Hilbert space of the system. Recently, so much attention has been directed to investigating ME versus BE in thermal states of many-body systems and their relative robustness to temperature, exploring the feasibility of achieving high temperature entangled states. The ME and BE properties in a 1D XYX spin model in an external field, using the Monte Carlo simulation, were investigated [41]. It was shown that the system possesses a factorized ground state [22] signalled by vanishing τ_1 and τ_2 and a quantum phase transition corresponding to an anomaly in the ratio R in the form of a narrow minimum versus the magnetic field. This suggests that the pairwise correlations suffer a big loss across the quantum critical point in contrary to ME which dominates and as a result, ME can be safely considered as the actual resource for the observed quantum phase transition. The minimum of the factor R was suggested as an estimator of the quantum critical points. Also a class of 1D XYZ spin systems, with different degrees of anisotropy, was shown to have factorizable ground states [24] where the pairwise entanglement range diverges while approaching these separable states, indicating a long range reshuffling of entanglement. At finite temperature, using τ_2 and concurrence, it was demonstrated that the system may emerge from a separable state into a mixed thermal entangled state with no pairwise entanglement present, i.e. containing only ME. The ME of a subsystem of three arbitrary spins in a 1D XY spin chain in an external magnetic field was evaluated [25], using the negativity between one spin and the other two [42]; compared with the BE of each pair of these three spins, it was shown that ME enjoys a longer range compared with BE through the chain. At finite temperature, it was demonstrated that ME is more robust than BE for a block of three adjacent spins where ME is still present, though there is no pairwise entanglement left in the system. Quite a few works have studied the quantification and behaviour of global ME in thermal states of many-body systems and mainly focused on systems possessing analytic solutions, such as 1D spin chains (e.g. [33, 35, 43]). To overcome the difficulties of evaluating the global entanglement in the thermal mixed states of many-body systems, there has been an approach to provide a transition temperature below which the ME is guaranteed in such systems based only on information about the ground state of the system and its partition function [33]. Using this approach, the robustness of ME in thermal states of the 1D spin-1/2 XY system was investigated and the threshold temperature for vanishing entanglement was estimated [35]. It was demonstrated that the threshold temperature increases monotonically with the magnetic field in the region of large values of the field. Due to the big computational difficulties, there is a lack in investigations in two-dimensional (2D) (and higher) quantum systems, with a few notable exceptions [44–48]. These works have focused on studying entanglement

in 2D finite and infinite square lattices using Monte Carlo simulations or the projected entangled-pair states [49]; they used concurrence, one tangle and fidelity to quantify ME and determine points of separable ground states and phase transitions at zero temperature.

In this paper, we consider two different systems of a finite number of spins, each in presence of an external transverse magnetic field in contact with a heat bath at temperature T. We provide an extensive investigation of a 2D XY spin-1/2-star model but also study a 1D XY spin-1/2 chain for the sake of comparison with the 2D system and the previous 1D results as well. The number of spins in each system is 7 and the nearest neighbour (nn) spins are coupled through an exchange interaction J. We investigate and compare the BE and the global ME of both systems under the effect of an external transverse magnetic field, thermal excitations and different degrees of anisotropy. We use the entanglement of formation and GE as measures of the bipartite and global MEs respectively. We show that, for both cases, in the anisotropic and partially isotropic systems at zero temperature, the MEs and BEs can be maintained at high magnetic field values where the nn and MEs assume very small values that are, however, still much higher than those of the next to nearest ones. Also we demonstrate that the threshold temperature, at which the entanglement vanishes, is higher for the nn entanglement compared to both of the next-to-nearest neighbour (nnn) BEs and MEs. Therefore, nn BE is more robust to thermal excitations compared to the next to nearest bipartite and global MEs in these systems. Also we demonstrated how an impurity can be used to tune and enhance the threshold temperature of all types of entanglement. We also examined the persistence of quantum effects at high temperatures by observing the entanglement behaviour and show that we may maintain non-zero entanglement at considerably high temperatures by applying strong enough magnetic fields.

This paper is organized as follows. In the next section, we present our model. In section 3, we focus on the 2D spin system and evaluate the BE and the thermal energy of the system. The ME and the threshold temperatures for all type of entanglements for the 2D system are evaluated in section 4. In section 5, we study impurity effects. In section 6, we calculate and compare the BE and MEs and the corresponding threshold temperatures in the 1D system. We conclude in section 7.

2. The Model

We consider two different systems, 2D and 1D spin-1/2 XY models with nn exchange coupling J subject to an external magnetic field h, with seven spins in each system. The first system is a 2D spin-star model consisting of one central spin and six surrounding spins, whereas the second system is a 1D spin chain, as shown in figure 1(a) and (b). The Hamiltonian of the system is given by

$$H = -\frac{(1+\gamma)}{2}\sum_{\langle i,j\rangle} J_{i,j}\sigma_i^x\sigma_j^x - \frac{(1-\gamma)}{2}\sum_{\langle i,j\rangle} J_{i,j}\sigma_i^y\sigma_j^y - h\sum_i \sigma_i^z, \quad (1)$$

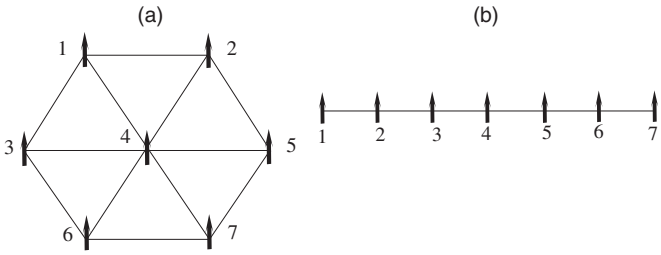

Figure 1. (a) 2D triangular spin lattice; (b) 1D spin chain.

where σ_is are the Pauli matrices, γ is the anisotropy parameter, $\langle i, j\rangle$ is a pair of nn sites on the lattice and $J_{i,j} = J$ for all sites. For this model, it is convenient to study a dimensionless Hamiltonian where we set $J = 1$ and define a dimensionless parameter $\lambda = h/J$. The Hilbert space of this spin systems is huge with 2^7 dimensions, nevertheless it can be exactly diagonalized using the standard computational techniques, yielding the system energy eigenvalues $\{E_i\}$ and eigenfunctions $\{\psi_i\}$. At absolute zero temperature, the system lies in its ground state $|\psi_0\rangle$, which is usually entangled with an amount that varies based on the values of the different system parameters. The system is described by the density matrix defined in terms of the pure ground state wavefunction $|\psi_0\rangle$ as

$$\rho = |\psi_0\rangle\langle\psi_0|. \quad (2)$$

Now, when the spin system is set into contact with a heat bath at an absolute temperature T, the system moves from its initial pure state, described by equation (2), to a mixed thermal state, which is a mixture of the ground state and a number N_e of excited states, represented by

$$\rho_T = \frac{1}{Z}\left\{e^{-\beta E_0}|\psi_0\rangle\langle\psi_0| + \sum_{i=1}^{N_e} e^{-\beta E_i}|\psi_i\rangle\langle\psi_i|\right\}, \quad (3)$$

where $\beta = 1/kT$, k is the Boltzmann constant and Z is the system partition function. The number of excited states involved depends on the temperature, where more states are added as the temperature is raised. This mixing of excited states with the ground state acts as a destructive noise that reduces the amount of entanglement contained in the system. When the temperature reaches a certain value, which varies based on the system characteristics and parameters values, the amount of noise created by the excited states due to thermal fluctuations is sufficient to turn the system into a disentangled state. This temperature is known as the threshold temperature, denoted by T_{th}, where below it the system is guaranteed to be entangled [33].

3. Thermal bipartite entanglement in 2D spin systems

To study the BE in the system, we confine our interest to the entanglement between only two spins, at any sites i and j [58]. All the information about the considered two sites i and j is contained in the reduced density matrix $\rho_{i,j}$, which can be obtained from the entire system's density matrix by integrating out all the spins states except i and j. We adopt the entanglement of formation as a well known measure of

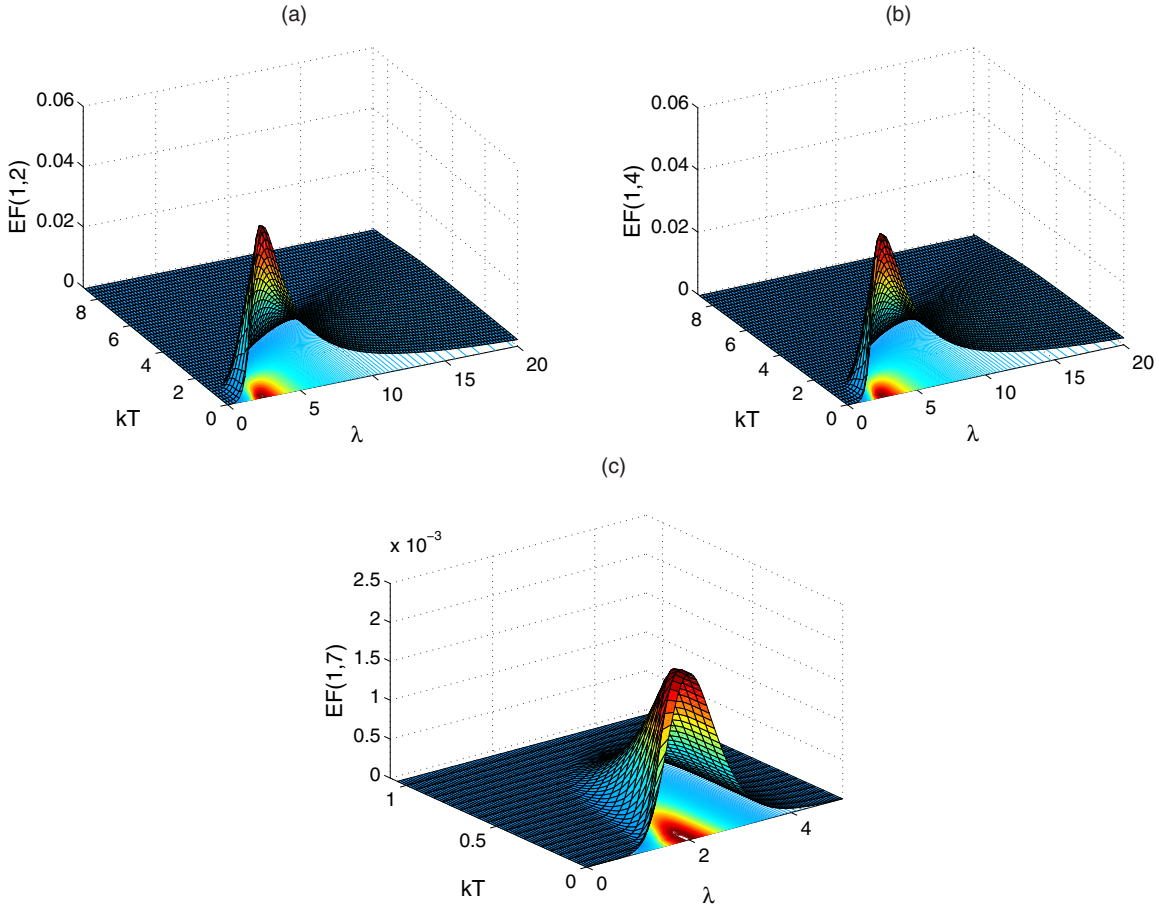

Figure 2. The BE EF(1, 2), EF(1, 4) and EF(1, 7) of the 2D Ising system ($\gamma = 1$) versus λ and kT(in units of J).

entanglement, where Wootters [29] has shown that, for a pair of binary qubits, the concurrence C, which goes from 0 to 1, can be used to quantify entanglement. The concurrence between two sites i and j is defined as

$$C(\rho_{i,j}) = \max\{0, \epsilon_1 - \epsilon_2 - \epsilon_3 - \epsilon_4\}, \tag{4}$$

where the ϵ_is are the eigenvalues of the Hermitian matrix $R \equiv \sqrt{\sqrt{\rho}\tilde{\rho}\sqrt{\rho}}$ with $\tilde{\rho} = (\sigma^y \otimes \sigma^y)\rho^*(\sigma^y \otimes \sigma^y)$ and σ^y is the Pauli matrix of the spin in the y direction. For a pair of qubits, the entanglement of formation is defined as,

$$\mathrm{E}(\rho_{i,j}) = \epsilon(C(\rho_{i,j})), \tag{5}$$

where ϵ is a function of C

$$\epsilon(C) = h\left(\frac{1 - \sqrt{1 - C^2}}{2}\right), \tag{6}$$

where h is the binary entropy function

$$h(x) = -x\log_2(x) - (1 - x)\log_2(1 - x). \tag{7}$$

In our calculations, we use the entanglement of formation EF as a measure of the BE. Using the mixed density matrix ρ_T defined in (3), one can evaluate the BE between any pair of spins in the system. In this section, we focus on studying the BE only in the 2D spin system sketched in figure 1(a). In figure 2, we have explored the behaviour of the entanglements of the nns EF(1, 2); EF(1, 4) and the next-to-next-to-nearest neighbour (nnnn) EF(1, 7) versus λ and the temperature kT for the anisotropic Ising system ($\gamma = 1$). In fact, the nnn EF(1, 5) is very close to EF(1, 7), as we will show below, but EF(1, 7) shows sharper changes, which makes us focus on it. As can be noticed, the nn BEs between two border sites EF(1, 2) and between a border site and the central one EF(1, 4) are strongest for very small magnetic fields but very fragile away from the zero temperature. On the other hand, as the magnetic field is increased, the entanglement maintains a small value which is more resistant to higher temperatures. Interestingly, the threshold temperature T_{th} at which the entanglement vanishes increases monotonically as the magnetic field increases. The (nnnn) entanglement EF(1,7) sustains only for very small values of the magnetic field and in the vicinity of the zero temperature; its value is much smaller than the nn entanglements. In order to further investigate the thermal robustness of the entanglement state and determine the magnitude of the entanglement precisely at high temperatures, we show the contour plot of the entanglements EF(1, 2), EF(1, 4) and EF(1, 7) in figure 3. As can be noticed, we can reach, for EF(1, 2) and EF(1, 4), a threshold temperature $kT = 8$ and higher by applying a magnetic field $h = 20$ and higher though the entanglement magnitude is very small. EF(1,7) is very fragile to temperature regardless of the strength of the applied magnetic field, as shown in figure 3(c).

The partially anisotropic system with $\gamma = 0.5$ was found to exhibit a close behaviour to the $\gamma = 1$ case, as depicted in figure 4. The peak of the entanglements, at a small magnetic

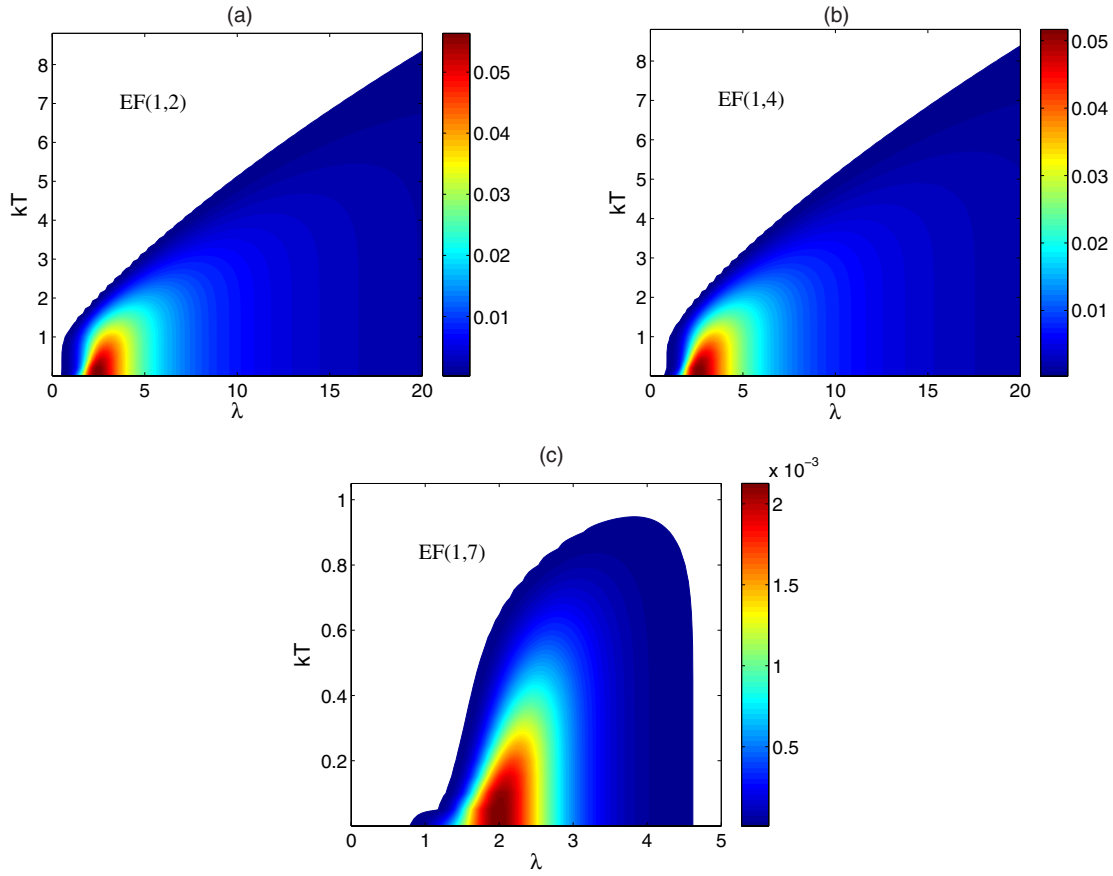

Figure 3. The contour plot of the BE EF(1, 2), EF(1, 4) and EF(1, 7) of the 2D Ising system ($\gamma = 1$) versus λ and kT(in units of J).

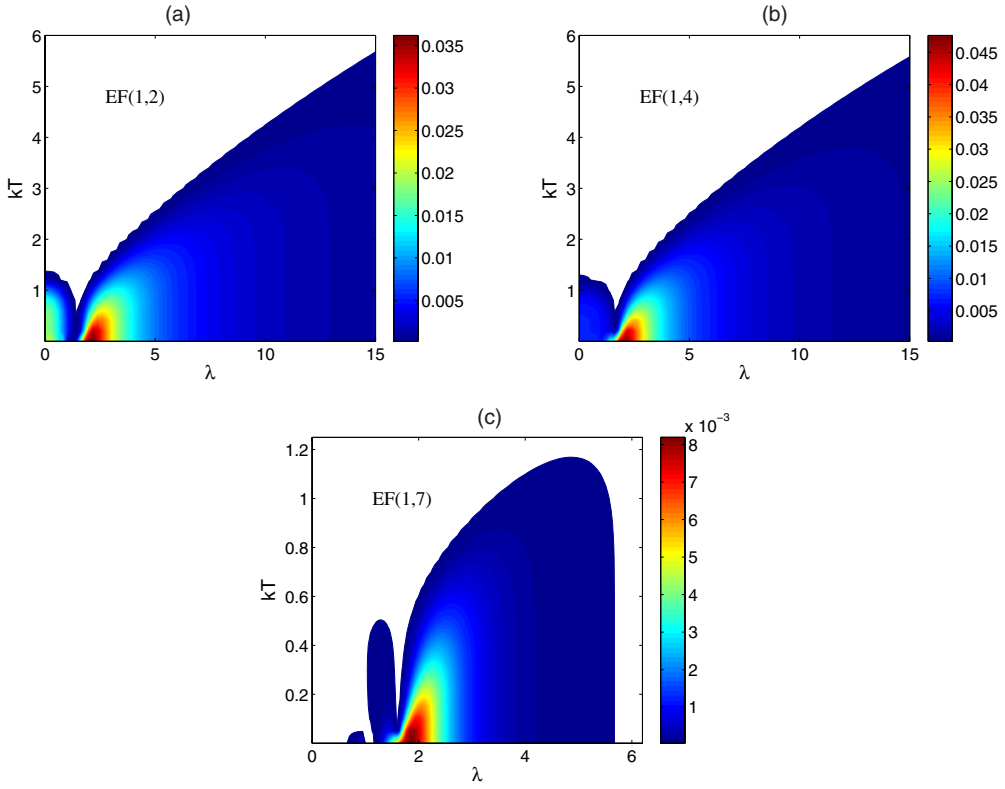

Figure 4. The contour plot of the BE EF(1, 2), EF(1, 4) and EF(1, 7) of the 2D partially anisotropic system ($\gamma = 0.5$) versus λ and kT(in units of J).

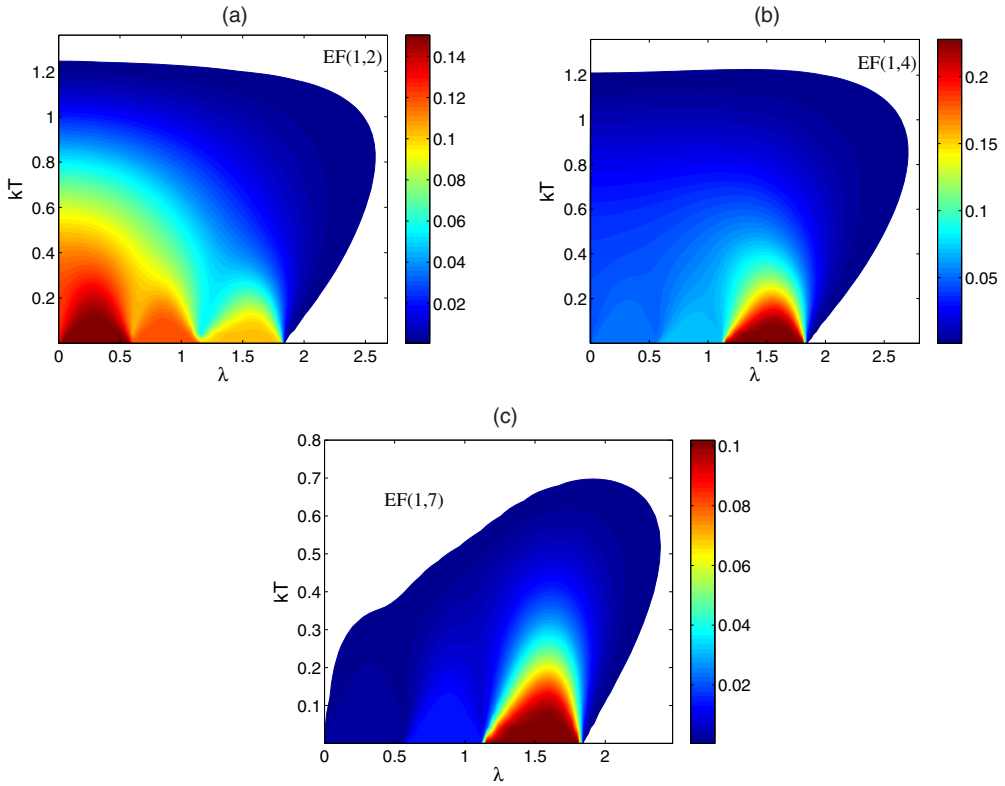

Figure 5. The contour plot of the BE EF(1, 2), EF(1, 4) and EF(1, 7) of the 2D isotropic system ($\gamma = 0.$) versus λ and kT(in units of J).

field and in the neighbourhood of zero temperature, is not single and this is due to the profile of the system's energy gap for $\gamma = 0.5$, as will be discussed in more detail below. It is clear that the value of the threshold temperature corresponding to the different magnetic field values is smaller compared to that of the $\gamma = 1$ case, as can be concluded from figures 3 and 4. Interestingly, the completely isotropic spin system with $\gamma = 0$ behaves in a completely different way compared to $\gamma = 0$ and 0.5, as shown in figure 5. As can be noticed from the figures, not only EF(1, 7) but also EF(1, 2) and EF(1, 4) vanish at very small temperatures, about a few kT. Clearly the thermal fluctuations are very devastating to the isotropic system where the BE over the whole lattice vanishes at a very small temperature. The peak of the entanglement EF(1, 2) is higher than that of EF(1, 4) but EF(1, 7) is much lower than both. In fact, this behaviour of the isotropic system ($\gamma = 0$) should not be very surprising, as it is known that the systems described by the Hamiltonian equation (1) at the thermodynamic limit belong to different universality classes based on the value of γ. The isotropic system is characterized by a separable state at a small value of the magnetic field; for the considered system at $\gamma = 0$, the ground state is separable for $\lambda \approx 1.85$ and higher.

In order to investigate the robustness of entanglement at much higher temperatures, we depict, as an example, the contour of the entanglements EF(1, 2) (at $\gamma = 1$), EF(1, 4) (at $\gamma = 0.5$), at a very high magnetic field in figures 6(a) and (b) respectively, which confirms the survival of entanglement, though very low in magnitude, at a high temperature. Interestingly, when we considered EF(1, 7) in the Ising system and the partially anisotropic system ($\gamma = 0.5$) at high magnetic fields and temperatures, we found that it is not exactly zero (only for $\gamma = 0.5$) though it is extremely small, as shown in figure 6(c).

It is of great interest to examine the relationship between the robustness of thermal entanglement and the corresponding thermal energy gap of the system. By the thermal energy gap, ΔE_{th}, we mean the difference between the mean (ensemble average) energy of the system at temperature T and the system's ground-state energy, i.e. $\Delta E_{\text{th}} = \langle E \rangle - E_0$. In figures 7(a)–(c), we present the contour plots of energy gaps for the systems with $\gamma = 1$, 0.5 and 0 respectively versus λ and kT for small values of λ. As can be seen, there are clear differences between the different cases, where the energy gap in the Ising system shows one sharp minimum before increasing montonically as λ increases, which gives rise to one corresponding sharp peak of entanglement in that case at the small values of λ. The energy gaps in the partially anisotropic and isotropic systems show two and multiple minima respectively before they also increase monotonically with λ, which causes the double peaks and multiple peaks, with different relative intensities, in the two systems respectively. This explains the different profiles of the entanglement peaks, at small values of the magnetic field, as the degree of anisotropy changes, as demonstrated in figures 3–5. On the other hand, the thermal energy gap at the different anisotropic values looks asymptotically (at a high magnetic field) the same, as shown in figure 7(d) for the case $\gamma = 0$, for instance.

Remarkably, one can see a strong correspondence between the strength and survival of entanglement, particularly for

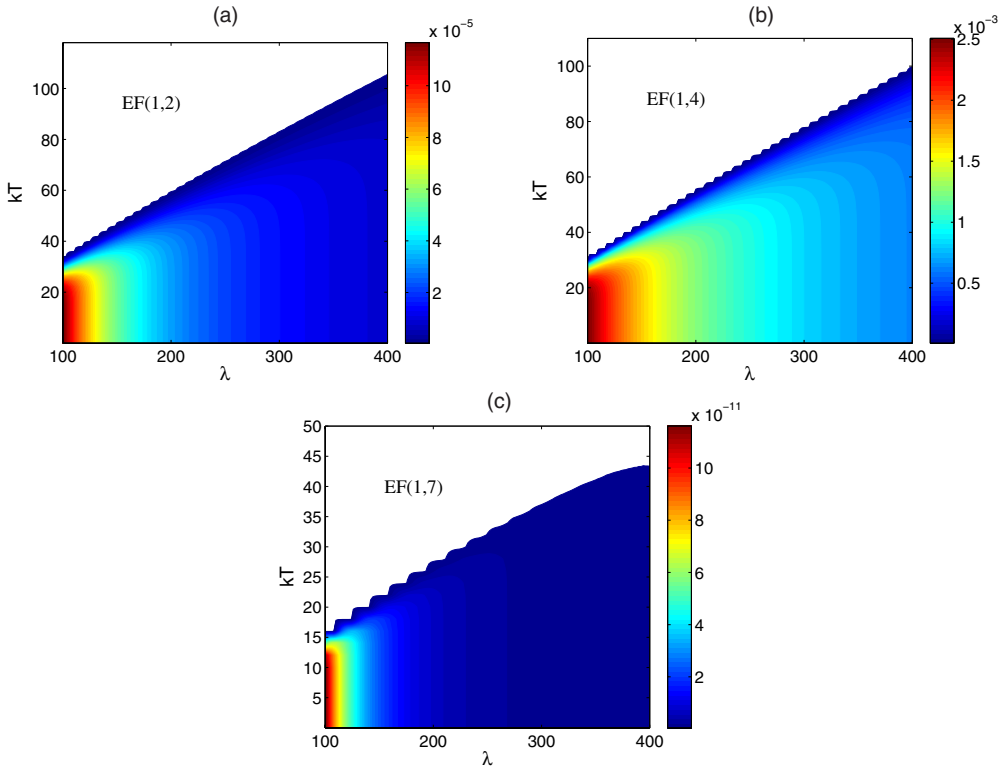

Figure 6. The contour plot of the BE (a) EF(1, 2) (for $\gamma = 1$); (b) EF(1, 4) (for $\gamma = 0.5$) and (c) EF(1, 7) (for $\gamma = 0.5$) of the 2D spin system versus λ and kT (in units of J) for a range of λ from 100 to 400.

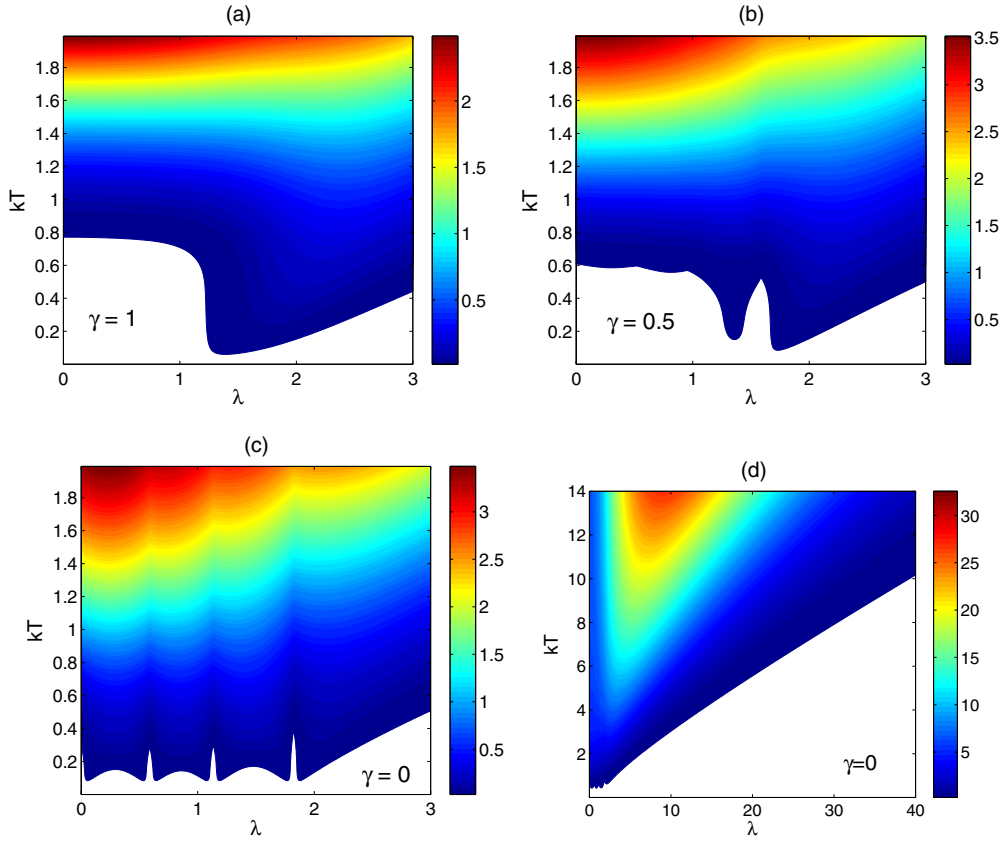

Figure 7. The contour plot of the thermal energy gap (in units of J) of the 2D spin system versus λ and kT (in units of J) for (a) $\gamma = 1$; (b) $\gamma = 0.5$; (c) $\gamma = 0$ and (d) $\gamma = 0$.

$\gamma = 0.5$ and 1 and the value of the energy gap when comparing figures 3, 4 and 7. The energy gap is either zero (the white regions of the contour plot) or quite small in the domains of non-zero entanglement. As can be noticed, the thermal energy gap increases monotonically as the magnetic field intensity increases, which explains the survival of the entanglement, despite its small magnitude, at relatively high temperatures and its strong resistance against thermal excitations compared to the high magnitude entanglement at the small values of the magnetic field, which is very fragile to temperature. It is important to emphasize here that though the energy gap profile looks asymptotically almost the same for the three anisotropic parameter values, nevertheless the entanglement in the isotropic system ($\gamma = 0$), contrary to the other two cases, vanishes at a very low temperature regardless of the energy gap value; this is due to the fact that this system's ground state, as we mentioned before, is disentangled for $\lambda \approx 1.85$ and higher.

4. Robustness of thermal entanglement in 2D spin systems

In order to study the ME of the entire lattice, a distance-like measure of entanglement, namely the global robustness of entanglement $R(\rho)$ [31, 33] is commonly used, which is defined for a general state ρ as the minimum amount of noise (t) needed to destroy the entanglement content of ρ and is given by

$$R(\rho) := \min_{\omega} \; t, \tag{8}$$

where ω is the state when added to ρ converts it to a separable state ϕ, such that

$$\phi(\omega, t) := \left\{ \frac{1}{1+t}(\rho + t\,\omega) \right\} \in S, \tag{9}$$

where S is the set of all separable states. The resultant separable state ϕ can be regarded as a mixture of two states, ρ and ω, with relative populations $1/(1+t)$ and $t/(1+t)$ respectively. This general approach can be applied, in particular, to a system in contact with a heat reservoir to determine the threshold temperature, $T_{\rm th}$, below it the system is guaranteed to be entangled [33]. Therefore, for instance in the spin system, if the state ρ is identified as the ground state ψ_0 and the rest of the states $\{\psi_i\}$, which get mixed with ψ_0 as the temperature is raised, as ω, then the population of the state ρ is given by $1/(1+t) = \mathrm{e}^{-E_0/kT}/Z$. As a result, the condition for the system to be guaranteed entanglement at a temperature T will read

$$\frac{\mathrm{e}^{-E_0/kT}}{Z} > \frac{1}{1+R(\psi_0)}, \tag{10}$$

where $R(\psi_0)$ is the global robustness of the ground state ψ_0, which has an energy eigenvalue E_0. To obtain the threshold temperature one has to turn the inequality in equation (10) into an equality and we get

$$\frac{\mathrm{e}^{-E_0/kT_{\rm th}}}{Z} = \frac{1}{1+R(\psi_0)}. \tag{11}$$

To determine the threshold temperature, $T_{\rm th}$, one has to evaluate the robustness of entanglement of the ground state $R(\psi_0)$, which is a very difficult task, where the entire system's Hilbert state has to be searched for the noise mixed state ω. However, it was found that a lower bound for the robustness of entanglement can be obtained [33] by evaluating the GE, $G(\psi_0)$, instead [14], which is easier to evaluate, where in general for any pure state ψ

$$\frac{1}{1+R(\psi)} \leqslant \frac{1}{2^{\,G(\psi)}}, \tag{12}$$

which would enable us to calculate a lower bound for the threshold temperature, where below it the system is guaranteed to be entangled. In all the figures, we simply denote this temperature as $T_{\rm th}$.

The geometric measure of ME utilizes the geometric properties of the Hilbert space to find the distance (or angle) between a pure state, ψ, representing the system and the closest pure separable state, ϕ to it, i.e. $||\ |\psi\rangle - |\phi\rangle\ ||$. The square sin of the angle between the two states ψ and ϕ represents a good measure of the global GE, where the smallest value of the square sine specifies the closest separable state to the pure state ψ and is defined by

$$G(\psi) := 1 - [\max_{\phi}\ ||\langle\psi|\phi\rangle||]^2, \tag{13}$$

where $||\langle\psi|\phi\rangle||$ represents cosine the angle between the two states ψ and ϕ. By evaluating the GE and using equations (11) and (12), we can find the lower limit of the threshold temperature $T_{\rm th}$.

In order to find the closest separable state to the state ψ, we assume an arbitrary separable state ϕ as a product of the single spin states of the seven spins, which takes the form

$$|\phi\rangle = \prod_{i=1}^{i=7} \left\{ P_i|0\rangle + \sqrt{1-P_i^2}\,\mathrm{e}^{\mathrm{i}\delta}|1\rangle \right\}. \tag{14}$$

Utilizing the reality of the wavefunction, where the eigenstates of this class of Hamiltonians are real, we set the azimuthal angle $\delta = 0$ [14, 18]. In addition, we have also examined numerically the independence of the results on the azimuthal angle. The set of parameters $\{P_i, i = 1, 2, \ldots 7\}$ has to be varied over its entire range to cover the whole system's Hilbert space searching for the closest distance between ψ and ϕ where $0 \leqslant P_i \leqslant 1$. Searching the entire Hilbert space is a computationally difficult task; therefore, we have tested around 4×10^6 different distinct set of values for the P's parameters, uniformally distributed over the system's Hilbert space, for the calculations of the GE.

In this section, we investigate only the 2D spin system. In figure 8, we compare the BEs EF(1, 2), EF(1, 4), EF(1, 5) and EF(1, 7) with the multipartite GE versus the parameter λ at zero temperature for different degrees of anisotropy. As can be noticed, the behaviour of the nnn entanglement EF(1, 5) is very close to the nnnn entanglement EF(1, 7) for all degrees of anisotropy. In figure 8(a), the nn BEs EF(1, 2) and EF(1, 4) of the Ising system after reaching its peak value at around $\lambda = 2.5$, decay as λ increases, whereas the nnn and nnnn BEs EF(1, 5) and EF(1, 7) reach exactly zero magnitude at small values of the magnetic field. On the other hand, the ME GE starts with a large magnitude, $\approx$0.92 at $\lambda = 0$, then decays abruptly as λ increases before it asymptotically approaches the nn entanglements, where all sustain with quite

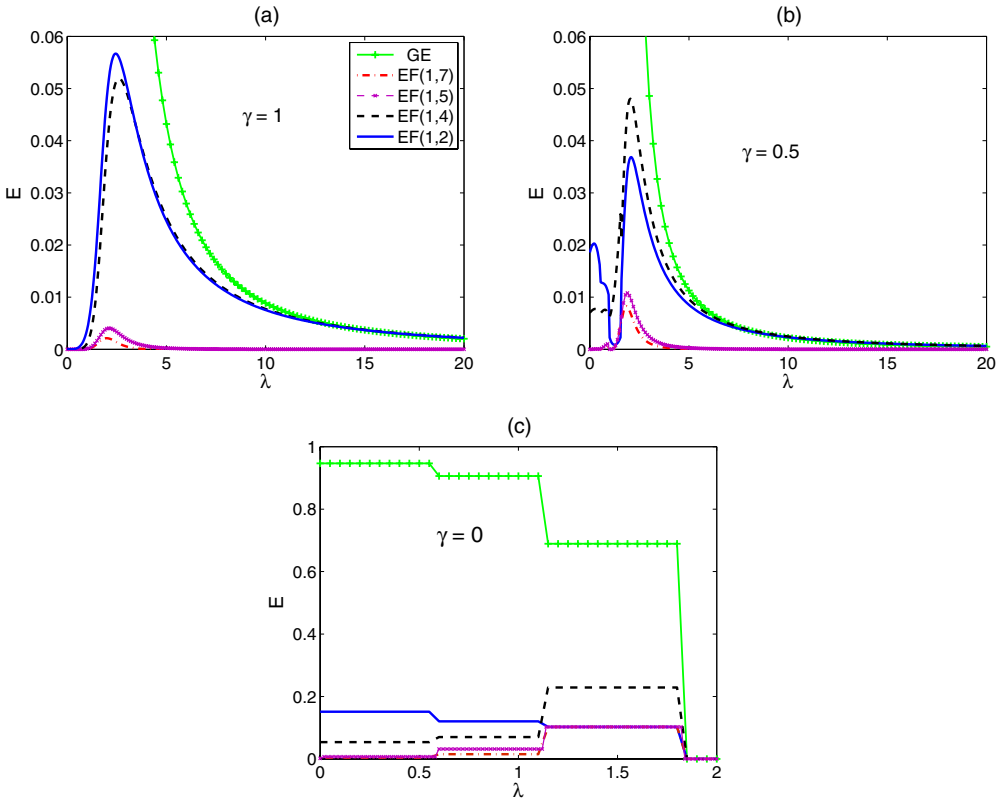

Figure 8. The entanglements EF(1, 2), EF(1, 4), EF(1, 5), EF(1, 7) and GE of the 2D spin system versus λ for $\gamma = 0,\ 0.5$ and 1 at zero temperature. The legends are as shown in subfigure (a).

small magnitudes up to large values of the magnetic field. In fact, examining the nn BE and GEs at a very large magnetic field strength shows that they reach quite small values that are of the same order of magnitude; for instance at $\lambda = 300$ they are of the order of 10^{-5}, though the magnitude of GE is always less than that of EF. A similar behaviour of the BEs and MEs is observed again in the partially anisotropic system, as shown in figure 8(b), but in this case, EF(1, 5) and EF(1, 7) sustain to a larger value of λ reaching very small magnitudes compared to EF(1, 2) and EF(1, 4). The behaviour of the entanglement in the isotropic system is depicted in figure 8(c) where all types of entanglement vanish at $\lambda \approx 1.85$; as we mentioned before, this stems from the fact that the ground state of the system is separable at this value and higher.

In figure 9, we compare the threshold temperature of the BEs, which is the temperature at which the BEs vanish, as was demonstrated in figures 3–5, to the threshold temperature of the ME, as defined before versus the parameter λ. In the Ising model, explored in figure 9(a), the threshold temperatures of the nn BEs EF(1, 2) and EF(1, 4) are very close and increase monotonically as the magnetic field increases. On the other hand, T_{th} for EF(1, 7) is very close to that of the GE at small values of the magnetic field where it increases monotonically but suddenly drops to zero around $\lambda = 6$, whereas T_{th} for the GE maintains its monotonic behaviour but is much smaller than T_{th} for EF(1, 2) and EF(1, 4). In figure 9(b), the threshold temperatures of the partially anisotropic system, $\gamma = 0.5$, behave in a similar way to the isotropic case where the temperatures for the nn BEs are very close; however, what is even more interesting is that the threshold temperatures for the nnnn BE sustains as the magnetic field increases and asymptotically becomes very close to that of the GE.

This means that the ME over the lattice along with the BE between the far spins (such as EF(1, 7)) are more fragile to temperature than the BE between the nn spins, such as EF(1, 2) and EF(1, 4), which manifests higher resistance and assumes a higher magnitude compared to GE and EF(1, 7) at the same temperature. A closer look at the behaviour of the threshold temperatures of the partially anisotropic system at small values of the magnetic field is given in figure 9(c). One can see sharp changes in the threshold temperatures especially for the nnnn entanglement and the GE, which can be explained in terms of the energy gap of the system, as will be discussed shortly. The threshold temperatures of the completely isotropic system, $\gamma = 0$, is explored in figure 9(d), where again the threshold temperatures of the nn entanglements EF(1, 2) and EF(1, 4) are very close and maintain an almost constant value before suddenly dropping to zero at $\lambda \approx 1.85$. The threshold temperature of EF(1, 7), which is considerably lower than that of the nns, increases linearly before suddenly dropping to zero also at the same value $\lambda \approx 1.85$. The threshold temperature of the ME exhibits an oscillatory behaviour with an average value within that of the nnnn bipartite value.

Figure 10 explains the sharp changes in the threshold temperatures at the small range of values of the magnetic field. As can be noticed in figures 10(a)–(c), the energy gap of the

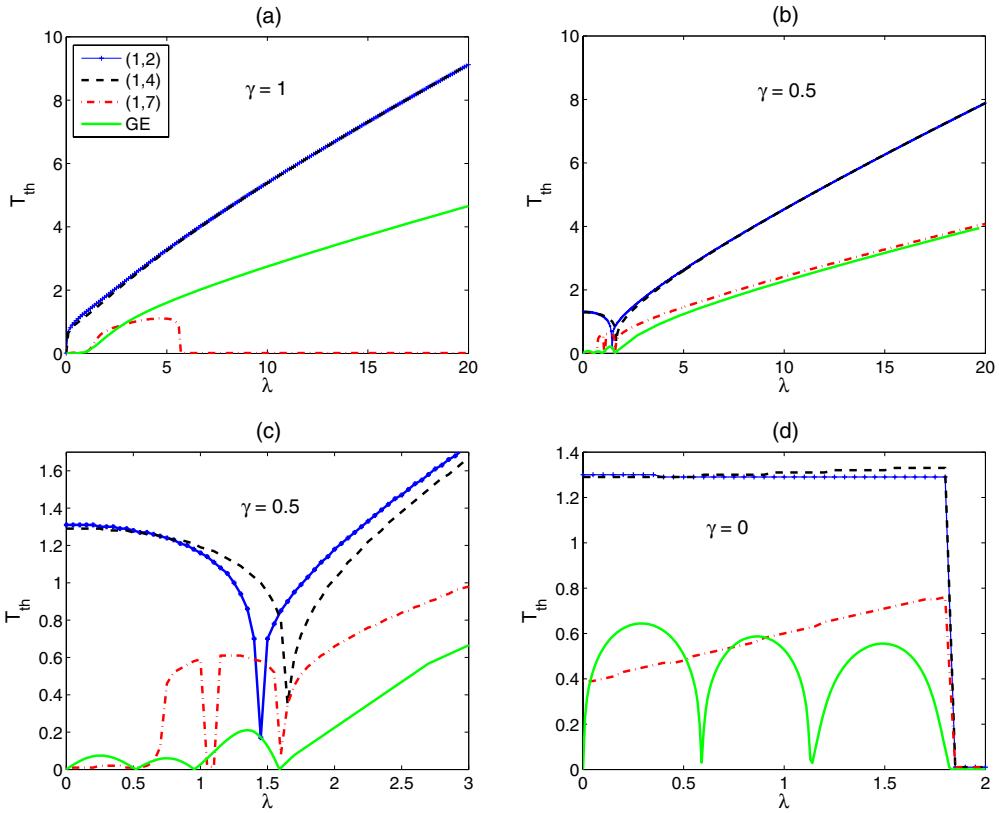

Figure 9. The threshold temperatures (in units of J) corresponding to the entanglements EF(1,2), EF(1,4), EF(1,7) and GE of the 2D spin system versus λ for $\gamma = 0,\ 0.5$ and 1. The legends are as shown in subfigure (a).

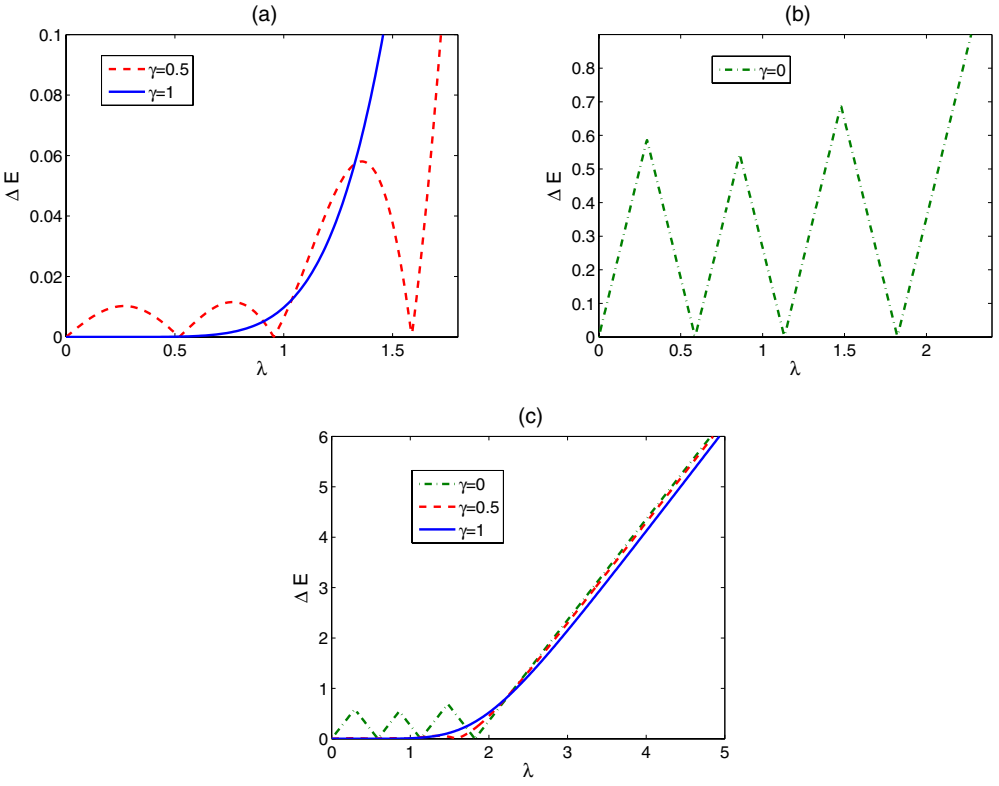

Figure 10. The energy gap (in units of J) of the 2D spin system versus λ for $\gamma = 0,\ 0.5$ and 1.

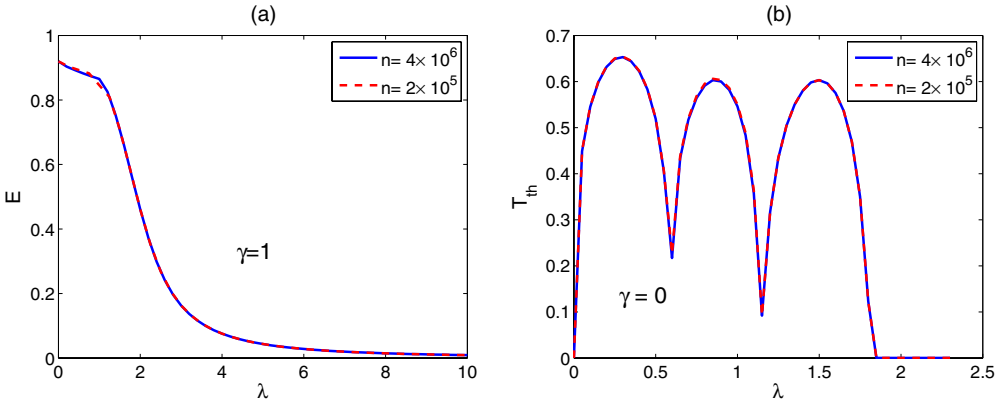

Figure 11. (a) The GE of the 2D Ising system ($\gamma = 1$) and (b) the threshold temperature (in units of J) of the 2D isotropic system ($\gamma = 0$), for two different numbers of the set of parameters $\{P_i\}$, $n = 2 \times 10^5$ and 4×10^6.

Ising system increases monotonically over the entire λ range with no sharp changes, which explains the smooth monotonic increase in the threshold temperatures shown in figure 9(a). In contrast, the energy gaps in the partially anisotropic and isotropic systems exhibit oscillating and sharp oscillating changes respectively at the small values of the parameter $\lambda \leqslant 1.85$ before coinciding with the anisotropic curve and increasing monotonically, as shown in figure 10. Interestingly, by comparing the behaviour of the threshold temperatures, particularly of the ME in figure 9, to that of the energy gaps in figure 10, one can notice the strict correspondence between them; the minima (and maxima) in the threshold temperatures coincide with that of the energy gaps on the parameter λ scale and when the energy gap increases monotonically, the threshold temperature follows that behaviour too. The impact of the energy gap on the ME is stronger compared to the BE due to the fact that the energy gap is calculated for the entire (multipartite) system. The effect of the number of the distinctive set of parameters $\{P_i, i = 1, 2, \ldots 7\}$ on the accuracy of the results is examined in figure 11 where two different numbers, 2×10^5 and 4×10^6, are compared in plotting the ME for $\gamma = 1$ and the threshold temperature for $\gamma = 0.5$, which shows a very strong coincidence.

5. Impurity effect

The imperfection and disorder in real physical systems have been always a big concern when studying the different quantum properties of many-body systems [21, 50]. Disorder and lack of homogeneity and isotropy cause a break of the translational symmetry and consequently the scaling of the entropy and all related quantities. An essential source of disorder is the presence of impurities in the physical system. The effect of quantum impurities in many-body systems and the quantification of the entanglement in these systems have been investigated [50]. The Von Neumann entropy was used to quantify the single site impurity entanglement in the considered systems. At finite temperature, the thermodynamic impurity entropy is used to quantify entanglement, especially in Kondo impurity systems [51, 52]. It was shown that the entanglement is significantly affected by the presence of the impurity even in the absence of physical coupling to the impurity itself. In a previous work, it was demonstrated that the entanglement and ergodicity in 2D spin systems can be tuned using impurities and anisotropy [53]. The effect of impurities on the spin relaxation rate [54] and dynamics of entanglement in 1D spin systems have been investigated [55]. The decay rate of the spin oscillation was found to be significantly affected by the coupling strength of the impurity spin.

In this section, we study the effect of a single impurity located at the central site on the threshold temperature of the different types of entanglement in the lattice. The single impurity is a spin that is coupled to its nns through an exchange interaction J', which differs from that between the other sites. We set $J' = (\alpha + 1)J$ where α is the impurity strength parameter. Here we consider three different cases for the impurity strength, $\alpha = -0.5, 0$ and 0.5 representing weak, null and strong ones respectively. In fact, such a system of seven spins with the central spin having a different coupling strength from the surrounding ones can be realized, for instance, in a system of coupled semiconductor quantum dots where the coupling between the valence electrons on the different dots is the exchange interaction, which can be controlled by raising or lowering the potential barrier between the dots [56].

In figures 12(a)–(c), we study the effect of the central impurity, with different strengths, in the 2D Ising lattice on the nn bipartite EF$(1, 2)$, nnnn bipartite EF$(1, 7)$ and the ME (GE) respectively. As can be noticed, the impurity strength has a minor effect on EF$(1, 2)$, where almost no change can be observed. Interestingly, in the case of EF$(1, 7)$, the critical value of the magnetic field at which the entanglement vanishes increases as the impurity strength increases. For strong impurity case, EF$(1, 7)$ never vanishes and increases monotonically as λ increases. This means that the impurity can be used to significantly preserve and enhance nnnn entanglement at a high temperature and magnetic field in the Ising system, which is also the case for GE, as can be noticed in figure 12(c). The partially anisotropic system is explored in figure 13. The impurity has a significant effect on EF$(1, 2)$ only at small values of λ, where it shifts the threshold minimum towards the right and creates an oscillation for a strong impurity value. The asymptotic value of EF$(1, 2)$ at large λ is not affected by the impurity strength. On the

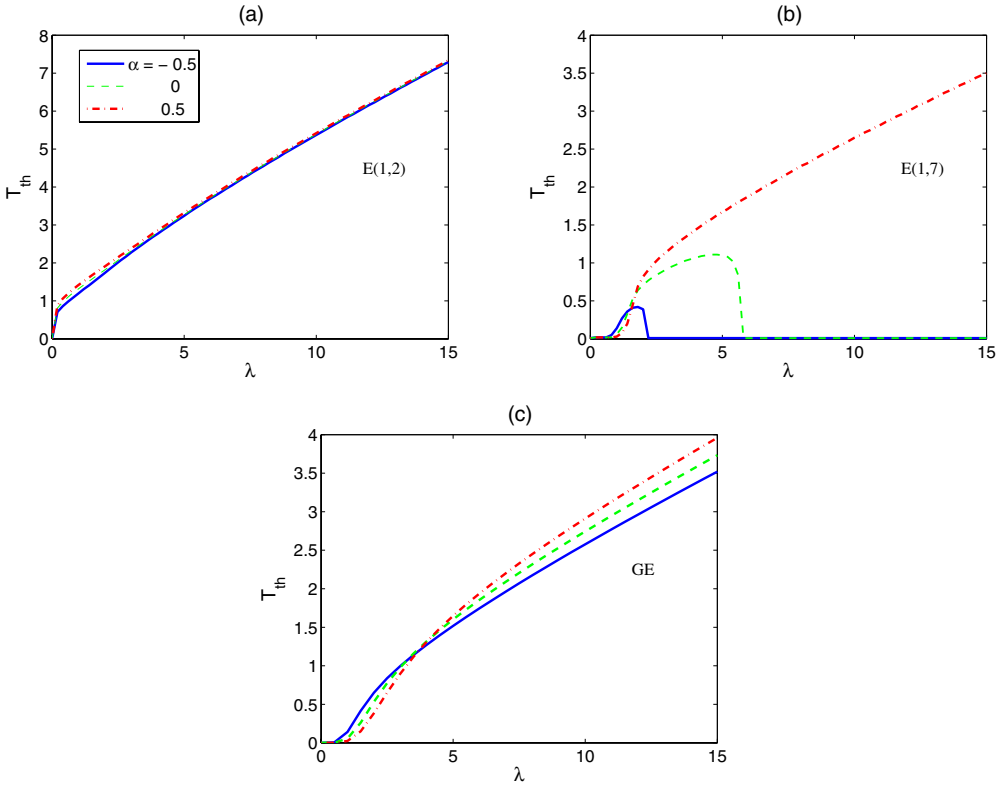

Figure 12. The threshold temperature of the entanglements EF(1,2), EF(1,7) and GE in the Ising 2D spin system with a central impurity versus λ at different impurity strengths. The legends are as shown in subfigure (a).

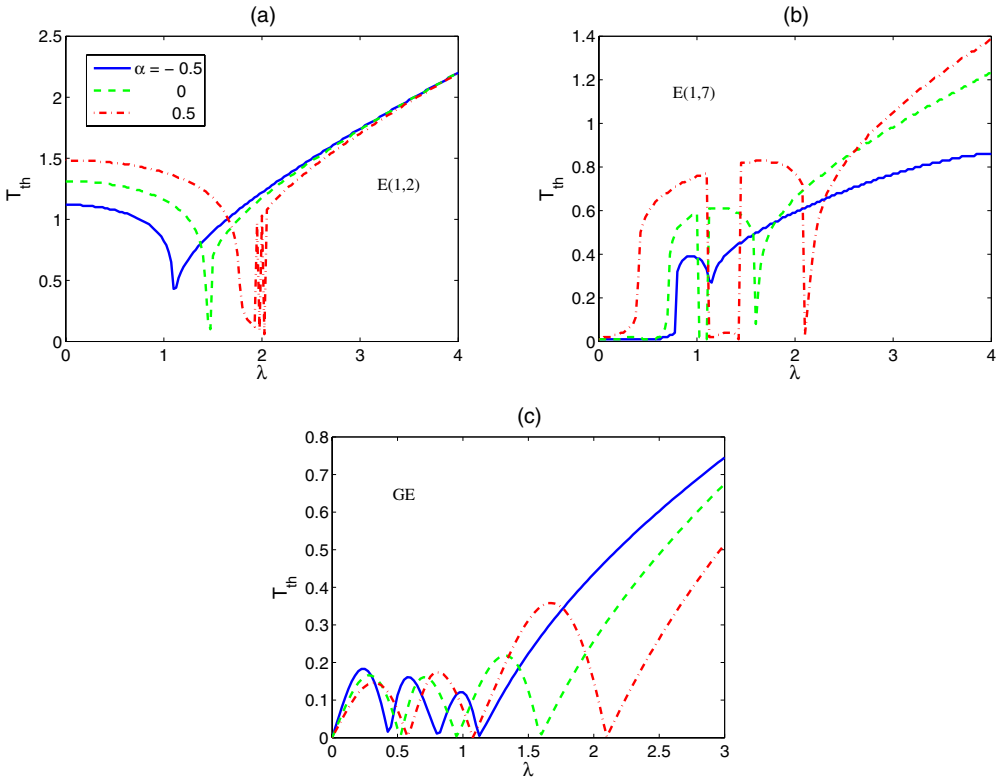

Figure 13. The threshold temperature of the entanglements EF(1,2), EF(1,7) and GE in the partially anisotropic 2D spin system with a central impurity versus λ at different impurity strengths. The legends are as shown in subfigure (a).

other hand, while the impurity strength enhances the nnnn asymptotic entanglement, it reduces the global entanglement but shifts the minima of T_{th} towards higher magnetic field values. The effect of the impurity on the isotropic system, with $\gamma = 0$, is shown in figure 14, where increasing the impurity strength clearly enhances all types of entanglement.

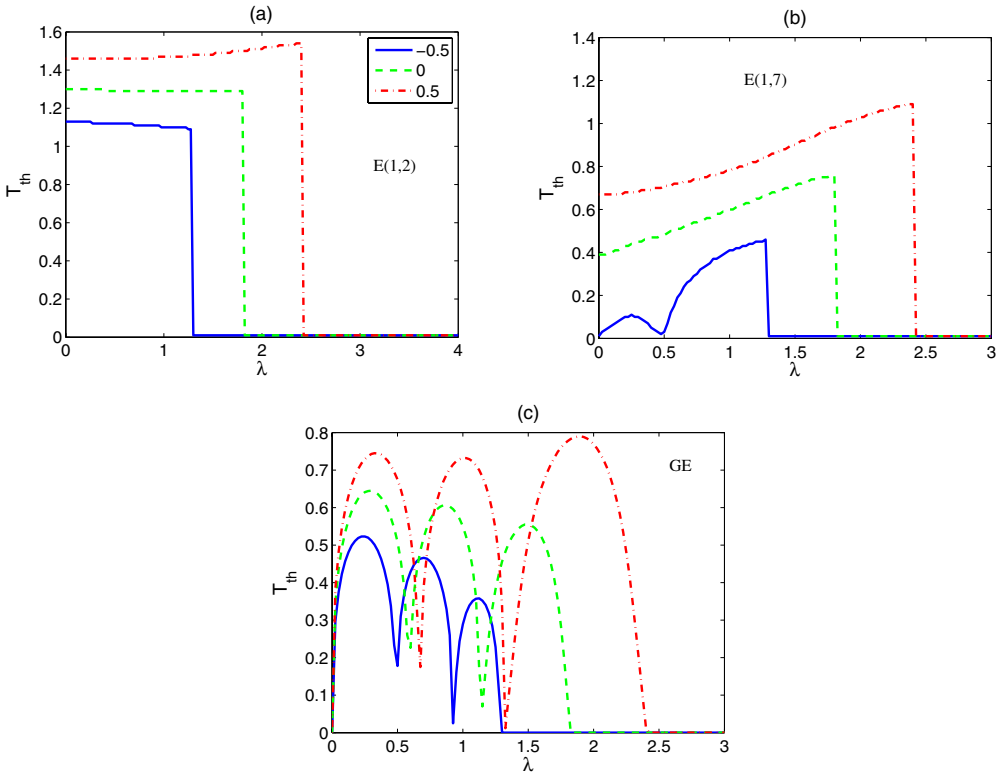

Figure 14. The threshold temperature of the entanglements EF(1,2), EF(1,7) and GE in the isotropic 2D spin system with a central impurity versus λ at different impurity strengths. The legends are as shown in subfigure (a).

In addition, it also shift the magnetic field critical value at which all entanglements vanish towards higher values. In fact, our results concerning the threshold temperatures here confirm the findings in a previous work [53] where it was shown that the entanglement can be enhanced or quenched in the spin system depending on the degree of anisotropy and the strength of the impurities.

6. Entanglements and threshold temperatures in 1D spin systems

Now let us consider a 1D *XY* spin chain consisting of seven spins, as sketched in figure 1(b), which is described by the same Hamiltonian equation (1) where, in this case, the exchange interaction $J_{i,j}$ exists only between each spin and its two nn spins on the chain. The system shows a close behaviour to what we have seen in the 2D case.

In figure 15(a), we compare the BEs to the ME for the Ising system, where, as can be seen, the nn entanglements EF(1, 2) and EF(2, 3) are very close as they start with zero magnitude at $\lambda = 0$ and increase as λ increases, reaching a maximum value around $\lambda = 1$ and then decay to zero at large λ. The nnn entanglement EF(1, 3) exhibits a similar behaviour but with a much smaller magnitude and in contrast to the 2D case, it sustains at large values of the magnetic field. The ME starts with a large value and abruptly decays approaching asymptotically the nn BEs at large magnetic field. The behaviour of the partially anisotropic system is very close to that of the Ising system, as shown in figure 15(b), except the quasi-oscillatory behaviour of the BE at values of $\lambda < 1$; however, again the nn bipartite and the GEs become close asymptotically, whereas the nnn entanglement sustains but with a much smaller magnitude. The entanglements of the isotropic system, similar to the 2D case, shows a step-like behaviour and vanish at the same point, which is $\lambda \approx 0.92$ in the current case, as depicted figures 15(c). The threshold temperature of the different types of entanglements in the 1D chain is explored in figure 16. Once more, the behaviour of the threshold temperatures of the nn entanglements EF(1, 2) and EF(2, 3) are close at the different degrees of anisotropy of the system and the case is the same for the nnn BE and MEs. Also, as can be seen, the isotropic system has zero threshold temperature at $\lambda \approx 0.92$. The behaviour of both the entanglements and threshold temperatures in the 1D spin chain can be explained in terms of the variation in the system's energy gap at zero temperature, which is depicted in figure 17. Similar to the 2D case, one can see the strict correspondence between the variations in entanglements and threshold temperatures and the variations in the energy gap for all degrees of anisotropy of the system and at all λ values.

Now, it is clear that the general behaviour of the MEs and BEs, in the one and 2D systems at the different degrees of anisotropy, shows that the threshold temperature of the system, considered at the same magnetic field, increases with γ within the range $0 < \gamma \leqslant 1$ and vanishes at a small value of the magnetic field for $\gamma = 0$. In addition, the threshold temperatures increase monotonically with the magnetic field for $\lambda \gg 1$.

In fact, our results, particularly the 1D case, are in complete agreement with the findings of [35], which is

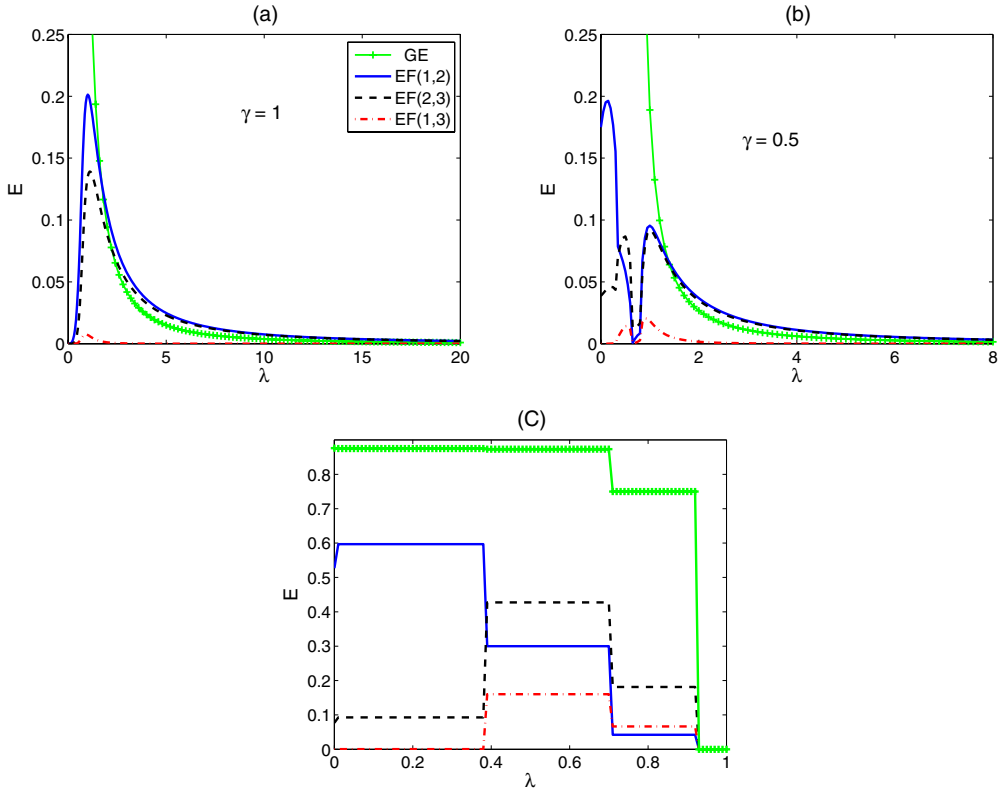

Figure 15. The entanglements EF(1,2), EF(2,3), EF(1,3) and GE of the 1D spin system versus λ for $\gamma = 0,\ 0.5$ and 1 at zero temperature. The legends are as shown in subfigure (a).

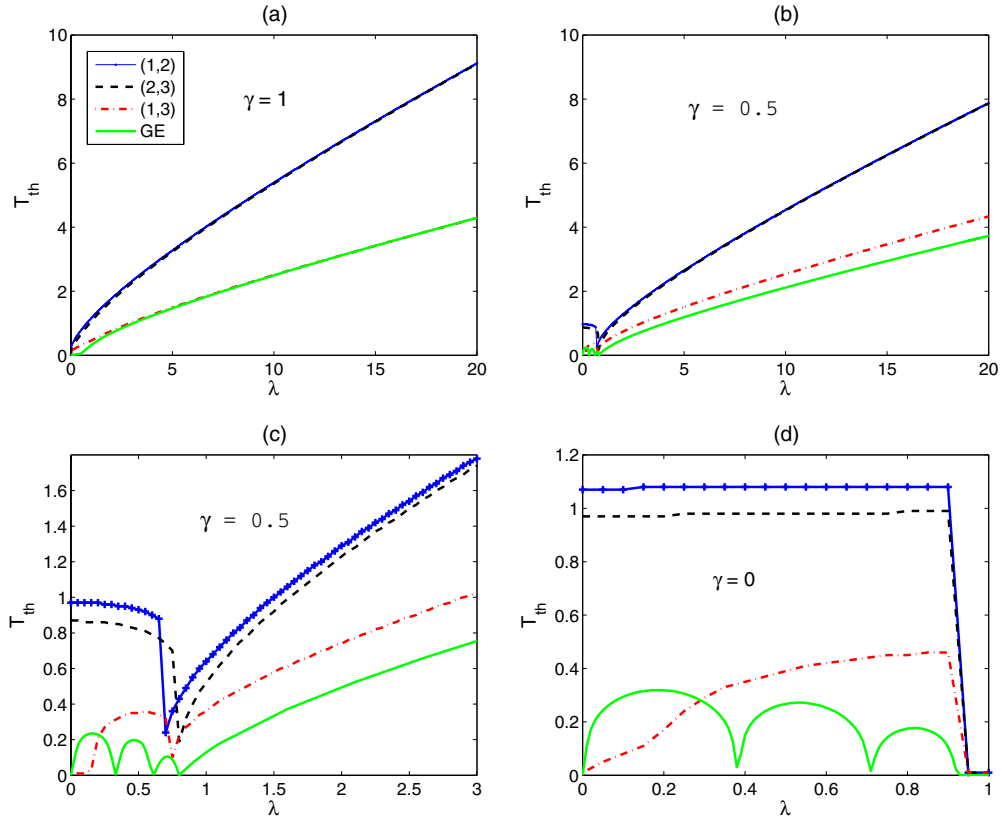

Figure 16. The threshold temperatures (in units of J) corresponding to the entanglements EF(1,2), EF(2,3), EF(1,3) and GE of the 1D spin system versus λ for $\gamma = 0,\ 0.5$ and 1. The legends are as shown in subfigure (a).

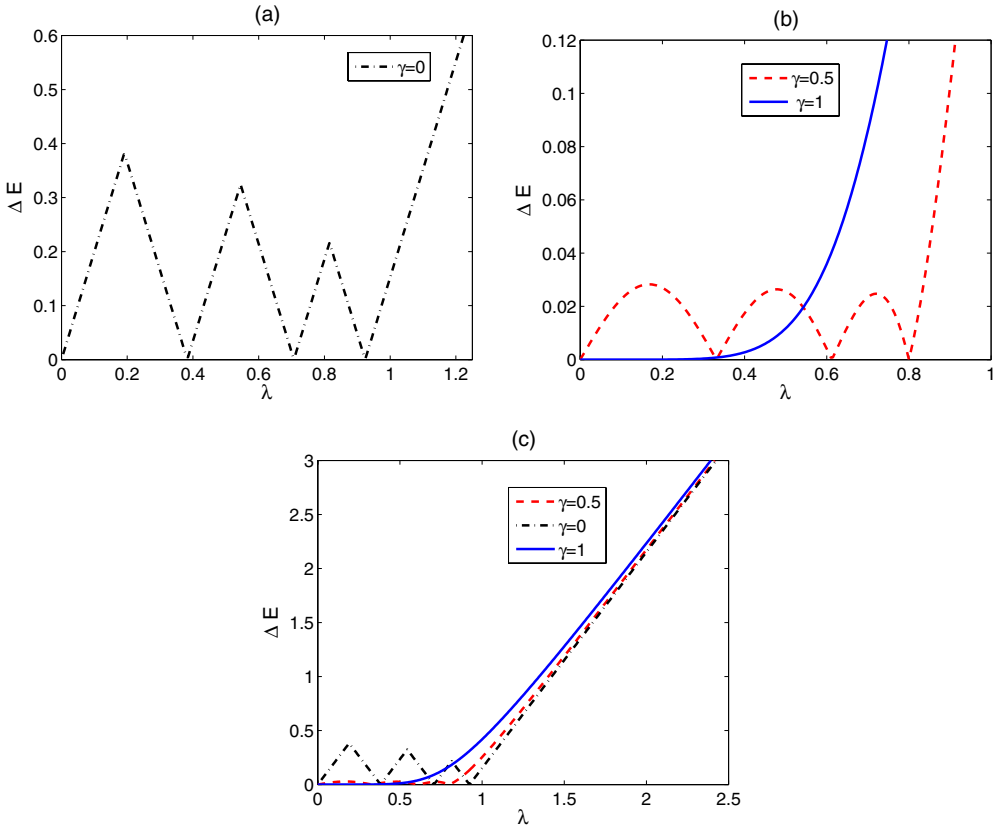

Figure 17. The energy gap (in units of J) of the 1D spin system versus λ for $\gamma = 0,\ 0.5$ and 1 at zero temperature.

concerned with the threshold temperature corresponding to the global entanglement in 1D XY model at different degrees of anisotropy (see figures 5 and 6 therein), though the results in those figures are for 80 spins. Also, our results agree with those of [25] concerning the monotonic behaviour and the relative magnitudes of nn to nnn of BE in the different pairs of three adjacent spins on a 1D isotropic XY spin chain utilizing the integrability of the model. However, the ME in their case, which is quantified using the negativity between one of the spins and the other two, shows a higher threshold temperature compared to that of BE in that case (see figure 3 therein). Furthermore, the minima that the entanglements go through at $\gamma = 0.5$, as presented in figures 8(b), 9(b), 9(c) and 15(b), bear resemblance to the findings of [22, 24] where minima of the entanglement were observed indicating the existence of factorizable (disentangled) ground states, which was also investigated in XYX spin systems [23, 45].

An estimate of the experimental values of the threshold temperatures for the typical spin systems of interest are due here. As the values of the threshold temperatures and energy gaps are all expressed in units of the exchange interaction constant J, which varies for the considered spin systems over a range of the order of μeV to meV [57], the corresponding range of the threshold temperature is 1.16×10^{-2} K to 11.6 K. Also, the typical value of the magnetic field h, which is also is expressed in units of J, can be evaluated here, which goes over the range 1.7×10^{-2} T to 17 T. Our results demonstrate that a bigger energy gap would lead to a higher threshold temperature but needs a stronger magnetic field too. Using these results, one can come up with important estimates, where, as can be concluded from figure 9, the 2D Ising system can reach a bipartite threshold temperature as high as 100 K, which needs a magnetic field that is as high as 300 T but the corresponding multipartite threshold temperature would be only about 50 K. The isotropic system is entangled up to a magnetic field of about 30 T where the maximum bipartite threshold temperature would be about 15 K and the maximum reachable multipartite threshold temperature is 7.5 K. For the same applied magnetic field, the threshold temperatures of the 1D spin chain would be slightly smaller than the corresponding ones in the 2D system as can be concluded from figure 16.

7. Quantum phase space of XY spin systems

Quantum phase transition in a many-body system happens either when an actual crossing takes place between the excited state and the ground state or a limiting avoided level crossing between them exists, i.e., an energy gap between the two states that vanishes in the infinite system size limit at the critical point [16]. When a many-body system crosses a critical point, significant changes in both its wavefunction and ground-state energy take place, which can be realized in the behaviour of the entanglement function and its derivatives [53, 58, 59]. It is well known that an infinite many-body system (i.e. at the thermodynamic limit) exhibits clear singularity at the critical point. However, finite sized systems may still show a strong tendency for being singular closer to the actual critical point of the system, which improves with the system size [53, 59].

The Hamiltonian equation (1) describes a family of models with different distinct phases at the thermodynamic limit ($N \rightarrow \infty$). The quantum phase diagram for the 1D system, in terms of γ and h, is well determined and contains three different phases: oscillatory, ferromagnetic and paramagnetic [60]. At the thermodynamic limit, the system reaches the isotropic and Ising limits at $\gamma = 1$ and 0 respectively. The system belongs to a universality class, the isotropic (XX) at $\gamma = 0$, whereas it belongs to a different class, Ising (aniostropic XY), in the range $0 < \gamma \leqslant 1$. The system possesses a quantum critical point at $\lambda = \lambda_c = 1$, where this point dictates the transition between different phases of the system depending on the value of γ. The system at all degrees of anisotropy exists in the paramagnetic phase for $\lambda > \lambda_c$. For $\gamma^2 + \lambda^2 < \lambda_c^2$ and $\gamma \neq 0$, the system exits in the oscillatory phase, whereas for $\gamma^2 + \lambda^2 > \lambda_c^2$ and $\lambda < 1$ is paramagnetic. The phase diagram of the infinite 2D system, though it is very similar to the 1D case, is not well established due to the lack of an analytic solution, computational difficulty and the different structures that the system may have. Many efforts have been directed to the prediction of the critical value of λ_c in the 2D spin system. For instance, the renormalization group method has been applied to the 2D infinite triangular (square) lattice and estimated a critical point at $\lambda_c = 4.757\,84(2.629\,75)$ [61], whereas the finite size scaling method applied to the square lattice predicts $\lambda_c = 3.044$ [62]. The point (with tendency to singularity) in the finite 2D spin system with 7-sites considered in this paper (and also for 19-sites), was estimated previously and found to be $\lambda_c = 1.64$ and 3.01 for the 7-sites and 19-sites systems respectively by studying the pairwise concurrence and its derivative in the system [59].

Though we emphasize here that the quantum phase transitions can take place only in the infinite system size (in the thermodynamic limit), we will try to draw a relation here between the behaviour of the entanglements and the threshold temperatures in our considered systems and the different phases of the system. As one can notice for the Ising system ($\gamma = 1$), the BEs have one single peak, where in fact its derivative locates the point of strong tendency for being singular [53, 59] before decaying monotonically with λ and the GE decay monotonically from a large value. This behaviour is reflected also in the threshold temperatures, which increase monotonically with λ. This profile of the entanglements and temperatures can be related to the transition from ferromagnetic to paramagnetic states for the Ising system as λ increases crossing the expected critical point. In the partially anisotropic system $\gamma = 0.5$, the entanglements (threshold temperatures) exhibit few maxima and minima with λ before monotonically decreasing (increasing), which can be explained in terms of the transition of the system from oscillatory to ferromagnetic and finally to the paramagnetic phase at the critical point. Finally, the isotropic system shows sharp changes in the entanglements (threshold temperatures)as they decay before vanishing at $\lambda \approx 1.85$, which can be explained in terms of the transition from the oscillatory phase to the paramagnetic phase; as we mentioned before, the vanishing of all entanglements and threshold temperatures is due to the fact that the isotropic system has a disentangled state for any magnetic field higher than this critical point.

8. Conclusions

We have investigated the robustness of bipartite and multipartite entanglement in 1D and 2D XY spin-1/2 lattices in an external magnetic field h against thermal excitations. The spins are coupled to each other through nearest neighbour exchange interaction J. The number of spins in the lattice is 7, which are coupled to a heat bath at temperature T. We have compared the bipartite entanglement to the multipartite entanglement versus the external applied magnetic field and temperature. Also, we compared the threshold temperature at which the entanglement vanishes in both cases. We used the entanglement as a measure of the bipartite entanglement and the geometric measure to evaluate the multipartite entanglement of the system.

In the 1D and 2D cases for the anisotropic and partially anisotropic spin systems at zero temperature, the nearest neighbour bipartite and multipartite entanglement can be maintained at large magnetic fields, though they would have very small values, which are still much higher than that of the next-to-nearest neighbour entanglements, except in the 2D Ising system where the latter vanishes at a small value of the field. In the isotropic system case, all types of entanglement vanish at the same small value of the magnetic field. The nearest neighbour bipartite threshold temperature was found to be higher than that of the next to nearest neighbour bipartite and multipartite where the temperatures of the last two get closer asymptotically and the three of them increase monotonically as the magnetic field increases. The exception is the threshold temperature of the nearest neighbour entanglement in the 2D Ising system, which vanishes at a small value of the magnetic field. Accordingly, the bipartite entanglement of the far spins of the system and the multipartite entanglement are less resilient towards thermal excitations compared to the nearest neighbour entanglement. All the threshold temperatures of the isotropic system vanish exactly at the same value of the magnetic field where all the entanglements vanish. Studying the different systems' energy gaps as a function of the magnetic field showed that they have great correspondence to the behaviour of the entanglements and the threshold temperatures, where large characteristic energy gaps lead to stronger robustness of entanglement and higher threshold temperatures, while vanishing energy gaps may cause zero threshold temperatures. Nevertheless, the properties of the ground state of the system plays a major role in determining the behaviour of the entanglement and the threshold temperature over the energy gap. This was particularly seen in the isotropic system case, which has a ground state that is entangled only below a threshold value of the magnetic field, which causes both the entanglement and the threshold temperatures to vanish at this value and above, regardless of the monotonic increase of the energy gap. The effect of a central impurity was found to be significant in enhancing the threshold temperatures and preserving all types of entanglements at high magnetic fields. Furthermore, we have focused on examining the persistence of quantum effects at high temperatures where we found that the different types of entanglements (especially the bipartite), though they would have very small values, can be

maintained at high temperatures by applying sufficiently high magnetic fields. It will be interesting in future to investigate the same systems coupled to a dissipative environment in the presence of thermal excitations to test the interplay of the two environments. Also, it is important to engineer similar systems with inserted impurities to examine their effect to tune the threshold temperatures. Furthermore, we would like to investigate the same system with a larger number of sites to test the system size effect on the robustness of thermal entanglement and determine threshold temperatures using finite size scaling [63, 64].

Acknowledgments

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