Bipartite entanglement in spin-1/2 Heisenberg model*

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Abstract The bipartite entanglement of the two- and three-spin Heisenberg model was investigated by using the concept of negativity. It is found that for the ground-state entanglement of the two-spin model, the negativity always decreases as B increases if $\Delta<\gamma-1$, and it may keep a steady value of 0.5 in the region of $B<J[(\Delta+1)^2-\gamma^2]^{1/2}$ if $\Delta>\gamma-1$, while for that of the three-spin model, the negativity exhibits square wave structures if γ=0 or Δ=0. For thermal states, there are two areas showing entanglement, namely, the main region and the sub-region. The main region exists only when $\Delta>\Delta_{\rm c}$ ($\Delta_{\rm c}=\gamma-1$ and $(\gamma^2-1)/2$ for the 2- and 3-spin model respectively) and extends in terms of B and T as Δ increases, while the sub-region survives only when $\gamma\neq 0$ and shrinks in terms of B and T as Δ increases.

Key words Heisenberg model, bipartite entanglement, negativity

PACS 03.67.-a, 03.67.Mn, 75.10.Jm

1 Introduction

Entanglement is an essential ingredient in the broad field of quantum mechanics, representing the nonlocal correlation between quantum systems that does not exist classically. Interest in entanglement in recent years mainly originates from its potential applications in the topical areas of quantum communication (QC) and quantum information processing (QIP)[1—3], such as quantum cryptography[1], teleportation[2], superdense coding[4] and quantum computation[5]. Naturally, as a promising resource for the implementation of entanglement, various types of quantum spin chains were introduced and analyzed extensively in the context of quantum information science[6—30], in particular their use as quantum wires[31—33] and as simple quantum processors[34].

The Heisenberg spin system, which may be a suitable candidate to simulate the relation between qubits in a quantum computer[35], is a simple but realistic and extensively studied solid-state system. The computational results of the preceding work show that the amount of the pairwise entanglement between two spins can be modified by varying the strength of the temperature or the external magnetic fields. In this paper, we study the properties of bipartite entanglement in the spin-1/2 Heisenberg model by applying the concept of negativity. We will consider only the two- and three-spin model, and concentrate on the dependence of entanglement on various parameters such as the external magnetic field, the anisotropic parameter as well as the temperature.

2 Formalism

In this section, we briefly recapitulate the definition of the negativity for a state ρ, which was firstly introduced by Vidal and Werner[36] and is defined as

$$\mathscr{N}(\rho)=\frac{\|\rho^{T_2}\|_1-1}{2}, \tag{1}$$

where the trace norm of ρ^{T_2} is equal to the sum of the absolute values of the eigenvalues of ρ^{T_2}, and T_2 denotes the partial transpose of ρ with respect to the second subsystem. The state ρ at thermal equilibrium is represented by the Gibb's density operator $\rho(T)=Z^{-1}\exp(-\hat{H}/k_{\rm B}T)$, where Z=tr$[\exp(-\hat{H}/k_{\rm B}T)]$ is the partition function, $k_{\rm B}$ is the Boltzmann's constant and is set to be 1 hereafter.

From the obvious fact that the partial transpose does not change the trace of a state ρ and tr(ρ)=1, it is direct to check that the negativity is equivalent to the absolute value of the sum of the negative eigenvalues of ρ^{T_2}, i.e.

$$\mathscr{N}(\rho)=\sum_i|\mu_i|, \tag{2}$$

Received 16 July 2007, Revised 16 November 2007

* Supported by National Natural Science Foundation of China (10547008)

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where μ_i is the negative eigenvalue of ρ^{T_2}.

The negativity has been shown to be an entanglement monotone, which can be computed efficiently. And obviously, it is a measure of the degree of violation of the Peres-Horodecki criterion in entangled states. Although this criterion is only a necessary separability condition, sufficient just for the case of two spin-halves and the case of (1/2,1) mixed spins, it fulfills some fundamental properties of an entanglement measure and bounds to the channel capacity and the distillable entanglement in quantum information processing.

In the special case that the state is pure $\rho=|\varphi\rangle\langle\varphi|$, with $|\varphi\rangle=a|00\rangle+b|01\rangle+c|10\rangle+d|11\rangle$, the above formula for the negativity can be simplified to

$$\mathscr{N}(\rho)=|ad-bc|. \tag{3}$$

3 Results and discussion

We consider the spin-1/2 Heisenberg XYZ model governed by the Hamiltonian

$$\hat{H} = J\sum_{i=1}^{L}\left[(1+\gamma)S_i^xS_{i+1}^x+(1-\gamma)S_i^yS_{i+1}^y+\Delta S_i^zS_{i+1}^z\right]+B\sum_{i=1}^{L}S_i^z, \tag{4}$$

where S^α ($\alpha=x, y, z$) denotes the spin-1/2 operator, $J(1+\gamma)$ and $J(1-\gamma)$ are the coupling in the x and y directions and $J\Delta$ is that in the z direction, γ and Δ are the anisotropic parameters with $\gamma\in[-1,1]$ and Δ is an arbitrary number. We constrict ourselves in this paper to the case of $\gamma\in[0,1]$ and $B\geqslant 0$ since changing the signs of γ and B has no intrinsic effect on the model.

3.1 The two-spin model

For the case of the two-spin model, if the periodic boundary condition (PBC) is imposed, then by applying the exact diagonalization method, the eigenvalues of the system are analytically obtained as

$$E_{1,2}=-\frac{1}{2}J\Delta\pm J,\quad E_{3,4}=\frac{1}{2}J\Delta\pm\eta, \tag{5}$$

with the corresponding eigenstates

$$\begin{aligned}|\phi\rangle_{1,2}&=\frac{1}{\sqrt{2}}(|01\rangle\pm|10\rangle),\\ |\phi\rangle_{3,4}&=\frac{1}{\sqrt{2\eta(\eta\pm B)}}\left[(B\pm\eta)|00\rangle+J\gamma|11\rangle\right],\end{aligned} \tag{6}$$

where $\eta=(B^2+J^2\gamma^2)^{1/2}$.

We first consider the ground-state entanglement, namely, the entanglement at zero absolute temperatures. From Eq. (5) it is direct to check that when η=0 (B=0, γ=0), the ground-state energy is E_2 if $\Delta>-1$, while it is $E_{3,4}$ if $\Delta<-1$ and $E_{2,3,4}$ if $\Delta=-1$. This gives the results $\mathscr{N}_{1\text{-}2}$=0.5 ($\Delta>-1$) and $\mathscr{N}_{1\text{-}2}$=0 ($\Delta\leqslant-1$), respectively. When $\eta\neq 0$, the ground-state energy is easily found to be

$$\begin{cases}E_2=-\frac{1}{2}J\Delta-J & (\text{if } \Delta>\eta/J-1)\\ E_{2,4}=-\frac{1}{2}\eta-\frac{1}{2}J & (\text{if } \Delta=\eta/J-1)\\ E_4=\frac{1}{2}J\Delta-\eta & (\text{if } \Delta<\eta/J-1)\end{cases}. \tag{7}$$

Thus for $\Delta>\eta/J-1$ the ground state is $|\phi\rangle_2$ and for $\Delta<\eta/J-1$, the ground state is $|\phi\rangle_4$, they are both pure states. However, for $\Delta=\eta/J-1$, $|\phi\rangle_2$ and $|\phi\rangle_4$ have the same energies, equal to the lowest energy of the system. In this case, we assume that the corresponding state is an equal mixture of $|\phi\rangle_2$ and $|\phi\rangle_4$, which can be shown properly by taking the zero-temperature limit of the thermal state $\rho(T)=Z^{-1}\exp(-\hat{H}/k_{\rm B}T)$. So based on the above consideration and according to the formalisms mentioned in Section 2, the negativity is obtained as

$$\mathscr{N}_{1\text{-}2}=\begin{cases}0.5 & (\text{if } \Delta>\eta/J-1)\\ \dfrac{\sqrt{2-\gamma^2/(\Delta+1)^2}-1}{4} & (\text{if } \Delta=\eta/J-1)\\ J\gamma/2\eta & (\text{if } \Delta<\eta/J-1)\end{cases}. \tag{8}$$

Clearly, if $\Delta<\gamma-1$, the negativity $\mathscr{N}_{1\text{-}2}$ always decreases with the increase of B, irrespective of γ. However, if $\Delta>\gamma-1$, there exists a critical magnetic field $B_{\rm c}=J[(\Delta+1)^2-\gamma^2]^{1/2}$ at which $\mathscr{N}_{1\text{-}2}$ becomes a nonanalytic function of B. The negativity $\mathscr{N}_{1\text{-}2}$ now initially keeps a steady value of 0.5 when B increases from B=0 to the neighborhood of $B<B_{\rm c}$, then when $B=B_{\rm c}$, $\mathscr{N}_{1\text{-}2}$ falls to a lower value of $(\sqrt{2-\gamma^2/(\Delta+1)^2}-1)/4$, which is due to the energy level crossing at this point. When $B>B_{\rm c}$, $\mathscr{N}_{1\text{-}2}$ decays off gradually as B increases. From Eq. (8) it is also easy to prove that when the anisotropy $\gamma>\gamma_{\rm c}=(\Delta+1)/5$, there occurs a revival of the bipartite

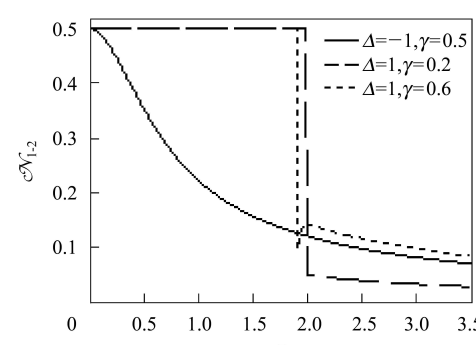

Fig. 1. The ground-state negativity $\mathscr{N}_{1\text{-}2}$ versus B for various anisotropic parameters γ and Δ.

entanglement for magnetic field B a little larger than B_c, as $\mathscr{N}_{1\text{-}2}$ in this case becomes larger than its value at $B=B_c$ (see Fig. 1). Moreover, it is also worthy to note that the critical value γ_c is different from that for the pairwise entanglement measure C, which is given by $(\Delta+1)/3$.

Let's now turn to the more realistic case of nonzero temperatures, i.e., the entanglement of thermal states. In the standard basis $\{|00\rangle, |01\rangle, |10\rangle, |11\rangle\}$, the partial transpose ρ^{T_2} can be written as

$$\rho^{T_2}=\frac{1}{Z}\begin{pmatrix} u_1 & & & m \\ & w & n & \\ & n & w & \\ m & & & u_2 \end{pmatrix}, \tag{9}$$

where

$$\begin{aligned} u_{1,2} &= \mathrm{e}^{-J\Delta/2T}[\cosh(\eta/T)\mp\frac{B}{\eta}\sinh(\eta/T)], \\ w &= \mathrm{e}^{J\Delta/2T}\cosh(J/T), \\ m &= -\mathrm{e}^{J\Delta/2T}\sinh(J/T), \\ n &= -\frac{J\gamma}{\eta}\mathrm{e}^{-J\Delta/2T}\sinh(\eta/T), \\ Z &= 2[\mathrm{e}^{J\Delta/2T}\cosh(J/T)+\mathrm{e}^{-J\Delta/2T}\cosh(\eta/T)]. \end{aligned} \tag{10}$$

Then using the exact diagonalization method, the eigenvalues of ρ^{T_2} are obtained as

$$\begin{aligned} \lambda_{1,2} &= \frac{w\pm n}{Z}, \\ \lambda_{3,4} &= \frac{u_1+u_2\pm\sqrt{(u_1-u_2)^2+4m^2}}{2Z}. \end{aligned} \tag{11}$$

From Eq. (10) it is easy to check that λ_2 and λ_3 are always positive, thus ρ^{T_2} has negative eigenvalues iff $w<-n$ or $u_1u_2<m^2$, which yields the following analytical expression of the negativity

$$\mathscr{N}_{1\text{-}2}=\max(0,-\lambda_1)+\max(0,-\lambda_4). \tag{12}$$

In Fig. 2 we show the negativities as functions of B and T for various anisotropic parameters γ and Δ, where J is chosen to be 1. When γ=0, Eq. (12) simplifies to $\mathscr{N}_{1\text{-}2}=\max(0, -\lambda_4)$ and the condition $u_1u_2<m^2$ becomes $\sinh(J/T)>\mathrm{e}^{-J\Delta/T}$. Clearly, the critical temperature T_c below which the entanglement exists is independent of the magnetic field B and only determined by the anisotropy Δ (cf. Fig. 2(a) and (b)), T_c increases as Δ increases. For the special case of Δ=0 and Δ=1, T_c can be obtained analytically as $T_{c1}=J/\ln(1+\sqrt{2})$ and $T_{c2}=2J/\ln 3$, respectively. From Fig. 2(a) and (b), it is also easy to see that the magnetic fields always suppress the bipartite entan-

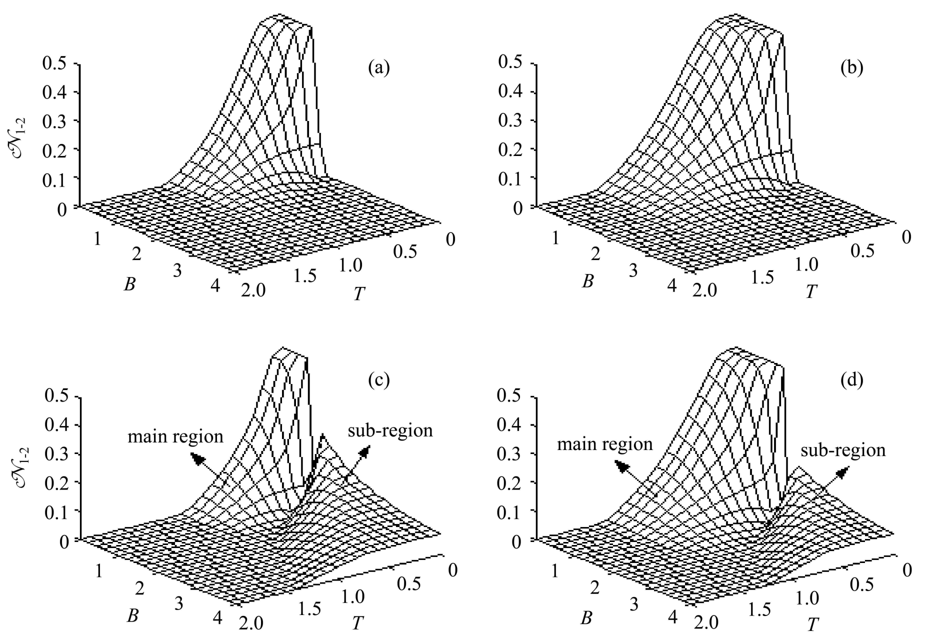

Fig. 2. The negativity $\mathscr{N}_{1\text{-}2}$ versus B and T for various anisotropic parameters γ and Δ. (a) γ=0, Δ=0; (b) γ=0, Δ=0.4; (c) γ=0.6, Δ=0; (d) γ=0.6, Δ=0.4.

glement when γ=0, and for higher values of B, the spins will be aligned, so there is no bipartite entanglement. When $B>J(\Delta+1)$, increasing temperature T may help to enhance the negativities. This behaviour is due to the fact that in region of $B>J(\Delta+1)$, the ground state at T=0 is the untangled state $|11\rangle$, and increasing T may bring the entangled states such as $|\phi\rangle_1$ and $|\phi\rangle_2$ into mixing with the ground state, thus the entanglement is enhanced.

When $\gamma\neq 0$, from Fig. 2(c) and (d) we notice that the region of nonzero negativity displays two distinct parts, which we define them the main region and the sub-region for the convenience of representation. The behaviors of $\mathscr{N}_{1\text{-}2}$ in the main regions are very similar to those of the γ=0 cases, while in the sub-regions, the thermal fluctuations always suppress the bipartite entanglement, and there exists a ridge of the negativity with the increase of B. When Δ increases after $\Delta+1>\gamma$, the main region is extended in terms of B and T, while the sub-region shrinks. When $\Delta+1\leqslant\gamma$, the main region disappears and only the sub-region remains. From the curve just detaching the nonzero and zero negativities on the B-T plane of Fig. 2(c) and (d), we also note that the critical temperature T_c here does not behave as a monotonic function of B and attains its minimum at about $B=J[(\Delta+1)^2-\gamma^2]^{1/2}$.

3.2 The three-spin model

For the three-spin model under periodic boundary condition, the eigenvalues are given by

$$\begin{aligned} E_{1,2} &= \frac{1}{4}J\Delta+\frac{1}{2}J+\frac{1}{2}B\pm\frac{1}{2}\eta_+, \\ E_{3,4} &= \frac{1}{4}J\Delta+\frac{1}{2}J-\frac{1}{2}B\pm\frac{1}{2}\eta_-, \\ E_{5,6} &= -\frac{1}{4}J\Delta-\frac{1}{2}J+\frac{1}{2}B, \\ E_{7,8} &= -\frac{1}{4}J\Delta-\frac{1}{2}J-\frac{1}{2}B, \end{aligned} \tag{13}$$

with the corresponding states explicitly expressed as

$$\begin{aligned} |\varphi\rangle_{1,2} &= \frac{1}{\sqrt{2\eta_+[\eta_+\pm(J\Delta-J+2B)]}}\times \\ &\left[(J\Delta-J+2B\pm\eta_+)|111\rangle+J\gamma\sum_{n=0}^{2}\mathscr{T}^n|010\rangle\right], \\ |\varphi\rangle_{3,4} &= \frac{1}{\sqrt{2\eta_-[\eta_-\pm(J\Delta-J-2B)]}}\times \\ &\left[(J\Delta-J-2B\pm\eta_-)|000\rangle+J\gamma\sum_{n=0}^{2}\mathscr{T}^n|110\rangle\right], \\ |\varphi\rangle_{5,6} &= \frac{\pm3-\sqrt{3}}{6}|110\rangle+\frac{\sqrt{3}}{3}|101\rangle+\frac{\mp3-\sqrt{3}}{6}|011\rangle, \\ |\varphi\rangle_{7,8} &= \frac{\pm3-\sqrt{3}}{6}|010\rangle+\frac{\sqrt{3}}{3}|100\rangle+\frac{\mp3-\sqrt{3}}{6}|001\rangle, \end{aligned} \tag{14}$$

where $\eta_\pm=[(J\Delta-J\pm2B)^2+3J^2\gamma^2]^{1/2}$, and $\mathscr{T}$ is the unitary cyclic right shift operator defined by its action on the basic $\mathscr{T}\ |m_1m_2m_3>=|m_3m_1m_2>$. Due to the complexity of the parameters involved, it turns out to be extremely tedious to give an analytical expression of the negativity for the three-spin model .So here we consider the ground-state entanglement of two special cases of γ=0 and Δ=0, respectively.

When γ=0, the model degenerates into the XXZ model, and there is no bipartite entanglement if $\Delta\leqslant-1/2$. If $\Delta>-1/2$, the negativity can be obtained as

$$\mathscr{N}_{1\text{-}23}=\begin{cases} 1/6 & (\text{if } B=0) \\ \sqrt{2}/6 & (\text{if } 0<B<B_{c1}) \\ (\sqrt{17}-3)/18 & (\text{if } B=B_{c1}) \\ 0 & (\text{if } B>B_{c1}) \end{cases}, \tag{15}$$

where $B_{c1}=J/2+J\Delta$, and the subscript 1-23 denotes the bipartition. Clearly, over the region between the two points B=0 and $B=B_{c1}$, the negativity displays a square wave structure, and out of this region, the bipartite entanglement disappears because the spins now are aligned parallel by the external magnetic fields.

When Δ=0, the model is the XY model, and from Eqs. (2), (13) and (14), it is easy to obtain that if γ=1 and B=0, there is no bipartite entanglement. For other cases, the negativity is given by

$$\mathscr{N}_{1\text{-}23}=\begin{cases} 1/6 & (\text{if } B=0,\gamma\neq1) \\ \sqrt{2}/6 & (\text{if } 0<B<B_{c2}) \\ \sqrt{2+2g^2}/(3+g^2) & (\text{if } B>B_{c2}) \end{cases}, \tag{16}$$

where g=$(J+2B+\eta_-)/J\gamma$ and $B_{c2}=J[(4-3\gamma^2)^{1/2}-1]/2$. Unfortunately, when $B=B_{c2}$, we cannot derive a simple analytic expression for the negativity. Except this point, $\mathscr{N}_{1\text{-}23}$ jumps from 1/6 to $\sqrt{2}/6$ in the vicinity of B=0, and maintains this constant value until $B>B_{c2}$, at which $\mathscr{N}_{1\text{-}23}$ decays off gradually with the increasing value of B.

It is worthwhile to note that the bipartite entanglement is nonzero for the three-qubit XY ($\gamma\neq1$) and XXZ models when B=0, in big contrast with the concurrence between a pair of qubits, which are always zero for the three-qubit XY and XXZ models. This phenomenon indicates that for these two models, even the ground state is not pairwise entangled, it still cannot be separated because it is bipartite entangled.

For finite temperatures, the negativities changing with B and T for different anisotropic parameters γ and Δ are shown in Fig. 3, where J is still set to be 1. One can see clearly that the magnetic field may help to enhance the bipartite entanglement for lower values of B and T, and except this region, the behaviors of the negativities are very similar to those of the two-spin cases, i.e., when γ=0, the critical temperature T_c has no relation with B and only increases with the increase of Δ (cf. Fig. 3(a) and (b)). Moreover, we may increase the entanglement by increasing T in the region of $B>J/2+J\Delta$. When $\gamma\neq0$, there are two different regions of the nonzero negativities, i.e., the main region and the sub-region. The main region extends in terms of B and T when Δ increases after $\Delta>(\gamma^2-1)/2$, while the sub-region shrinks in terms of B and T as Δ increases.

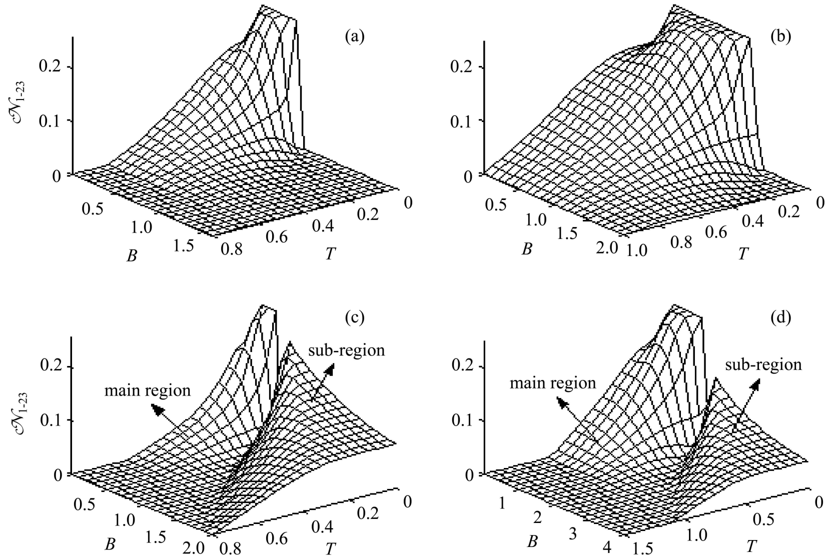

Fig. 3. The negativity $\mathscr{N}_{1\text{-}23}$ versus B and T for various anisotropic parameters γ and Δ. (a) γ=0, Δ=0; (b) γ=0, Δ=0.8; (c) γ=0.6, Δ=0; (d) γ=0.6, Δ=0.8.

4 Conclusions

In conclusion, we have investigated the properties of the bipartite entanglement in the two- and three-spin Heisenberg model by applying the concept of negativity. A general result is found that for the two-spin model, the ground-state negativity always decreases with the increase of B if $\Delta < \gamma - 1$, and it may keep a constant value of 0.5 in the region of $B < J[(\Delta+1)^2 - \gamma^2]^{1/2}$ if $\Delta > \gamma - 1$. For thermal entanglement, we show that when γ=0, one may increase the bipartite entanglement by increasing T in the region of $B > J(\Delta+1)$, and when $\gamma \neq 0$, there are two distinct regions of the nonzero negativities, i.e., the main region and the sub-region. The main region extends in terms of B and T when Δ increases after $\Delta+1 > \gamma$, while the sub-region shrinks.

For the three-spin model, we only consider the ground-state entanglement of the cases of γ=0 and Δ=0, and the results show that there are square wave structures in the negativities. For thermal states, the behaviors of the negativities are very similar to those of the two-spin cases, except that the main region exists only when $\Delta > (\gamma^2-1)/2$, and in the main region, the magnetic field may help to enhance the bipartite entanglement for lower values of B and T.

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