Thermal entanglement in one-dimensional Heisenberg quantum spin chains under magnetic fields

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The thermal pairwise entanglement (TE) of the $S=1/2$ XY chain in a transverse magnetic field is exactly resolved by means of the Jordan-Wigner transformation in the thermodynamic limit $N\to\infty$. It is found that the TE vanishes at a fixed point with temperature $T_c \simeq 0.484\,3J$, which is independent of the magnetic field. A thermal quantity is proposed to witness the entangled state. Furthermore, the TE of the $S=1/2$ antiferromagnetic-ferromagnetic (AF-F) Heisenberg chain is studied by the transfer-matrix renormalization-group method. The TEs of the spins coupled by AF and F interactions are found to behave distinctively. The vanishing temperature of the field-induced TE of the spins coupled by F interactions is observed dependent on the magnetic field. The results are further confirmed and analyzed within a mean-field framework.

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Quantum entanglement describes intrinsic correlations incurred in quantum mechanics. It plays the essential role in quantum information [1], quantum teleportation [2], and quantum cryptography [3]. In condensed-matter physics, it provides a new perspective to understand the collective phenomena in many-body systems [4].

The spin entanglement in quantum spin chains is of particular interest. Many types of entanglement at both zero and finite temperatures have been extensively studied in various spin systems (see reviews in Ref. [4]). As the finite-temperature entanglement [thermal entanglement (TE)] can be witnessed theoretically [5] and detected experimentally [6] by macroscopic variables, most efforts have been made to quantify the TE. The critical temperature (CT) below which the TE survives can even be estimated in experiment [7]. Interestingly, the numerical calculations indicate that the CT of the nearest-neighbor TE is a fixed point which is independent of the magnetic field in the $S=1/2$ Heisenberg chain [8] and two-qubit XY spins [9]. However, the features at the fixed point are unclear and no explanation exists. It is also a question whether the magnetic field independence of the CT is a universal phenomenon in quantum spin chains or there are exceptions. For these questions, in this paper, the field dependence of the CT of TE in the $S=1/2$ XY and antiferromagnetic-ferromagnetic (AF-F) Heisenberg chains are exactly resolved and studied by means of the transfer-matrix renormalization-group (TMRG) method in the thermodynamic limit $N\to\infty$, respectively. An analysis will also be made within the mean-field framework.

The pairwise entanglement of two $S=1/2$ spins at sites i and j in the ground state and at finite temperature can be achieved from the corresponding reduced density matrix $\hat{\rho}_{i,j}$, which, in the standard basis $\{|\uparrow\uparrow\rangle,|\uparrow\downarrow\rangle,|\downarrow\uparrow\rangle,|\downarrow\downarrow\rangle\}$, can be expressed as

$$\hat{\rho}_{i,j}=\begin{pmatrix} \langle P_i^{\uparrow}P_j^{\uparrow}\rangle & \langle P_i^{\uparrow}\sigma_j^{-}\rangle & \langle \sigma_i^{-}P_j^{\uparrow}\rangle & \langle \sigma_i^{-}\sigma_j^{-}\rangle \\ \langle P_i^{\uparrow}\sigma_j^{+}\rangle & \langle P_i^{\uparrow}P_j^{\downarrow}\rangle & \langle \sigma_i^{-}\sigma_j^{+}\rangle & \langle \sigma_i^{-}P_j^{\downarrow}\rangle \\ \langle \sigma_i^{+}P_j^{\uparrow}\rangle & \langle \sigma_i^{+}\sigma_j^{-}\rangle & \langle P_i^{\downarrow}P_j^{\uparrow}\rangle & \langle P_i^{\downarrow}\sigma_j^{-}\rangle \\ \langle \sigma_i^{+}\sigma_j^{+}\rangle & \langle \sigma_i^{+}P_j^{\downarrow}\rangle & \langle P_i^{\downarrow}\sigma_j^{+}\rangle & \langle P_i^{\downarrow}P_j^{\downarrow}\rangle \end{pmatrix}, \tag{1}$$

where $P^{\uparrow}=\frac{1}{2}(1+\sigma^z)$, $P^{\downarrow}=\frac{1}{2}(1-\sigma^z)$, and $\sigma^{\pm}=\frac{1}{2}(\sigma^x \pm \sigma^y)$. The brackets denote the ground-state and thermodynamic average values at zero and finite temperatures, respectively, and σ are Pauli matrices. As the phenomenon that is of interest mainly exists in the nearest-neighbor TE, we shall concentrate only on $\hat{\rho}_{i,i+1}$ in the following.

The spin operators can be transformed into spinless fermions by the Jordan-Wigner (JW) transformation

$$S_i^{+}=c_i^{\dagger}\exp\left(i\pi\sum_{j<i}c_j^{\dagger}c_j\right),\quad S_i^{z}=\left(c_i^{\dagger}c_i-\frac{1}{2}\right), \tag{2}$$

where $c_i^{\dagger}$ and c_i are the creation and annihilation operators of the spinless fermion, respectively. $\hat{\rho}_{i,i+1}$ becomes

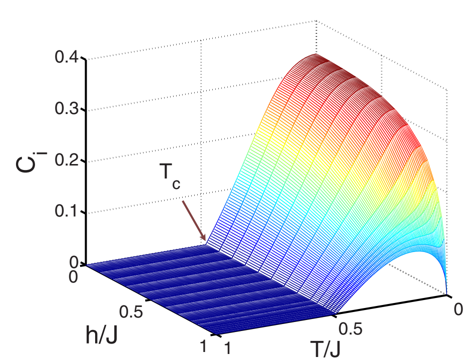

FIG. 1. (Color online) Temperature and magnetic field dependence of the thermal entanglement in the $S=1/2$ XY chain. The entanglements vanish at a common temperature T_c.

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$$\hat{\rho}_{i,i+1} = \begin{pmatrix} X_i^+ & 0 & 0 & 0 \\ 0 & Y_i^+ & Z_i^* & 0 \\ 0 & Z_i & Y_i^- & 0 \\ 0 & 0 & 0 & X_i^- \end{pmatrix}, \quad (3)$$

where $X_i^+=\langle n_i n_{i+1}\rangle (n_i \equiv c_i^\dagger c_i)$, $Y_i^+=\langle n_i(1-n_{i+1})\rangle$, $Y_i^-=\langle n_{i+1}(1-n_i)\rangle$, $Z_i=\langle c_i^\dagger c_{i+1}\rangle$, and $X_i^-=1-\langle n_i\rangle-\langle n_{i+1}\rangle+\langle n_i n_{i+1}\rangle$. As defined, the concurrence of TE of two nearest neighbors is given through

$$\tilde{C}_i = \mu_1 - \mu_2 - \mu_3 - \mu_4, \quad (4)$$

$$C_i = \max\{0,\tilde{C}_i\}, \quad (5)$$

where μ_i are the square roots of the eigenvalues of $\rho_{i,i+1}\tilde{\rho}_{i,i+1}$, where μ_1 is the largest. $\tilde{\rho}_{i,i+1}$ is a transformed matrix of $\rho_{i,i+1}$, i.e., $\tilde{\rho}=\sigma_y\otimes\sigma_y\rho^*\sigma_y\otimes\sigma_y$. Thus, Eq. (4) is transformed into

$$\tilde{C}_i = 2(|Z_i| - \sqrt{X_i^+ X_i^-}). \quad (6)$$

The concurrence can be calculated from the local-density, hopping term, and site-site correlations of the fermions.

As the observed field independence of the CT of TE is obtained by either numerical calculations [8] or only for two qubits [9], a deep understanding is indeed necessary. Therefore, we shall exactly resolve the concurrence of the $S=1/2$ XY chain in a transverse magnetic field within the thermodynamic limit to investigate this phenomenon analytically. The Hamiltonian of the $S=1/2$ XY chain is given as

$$H = \sum_{i=1}^{N} \frac{1}{2} J(S_i^+ S_{i+1}^- + \text{H.c.}) - h\sum_{i=1}^{N} S_i^z, \quad (7)$$

where $J(>0)$ is the coupling, and h is the magnetic field. As the XY chain with F couplings can be obtained by a unitary transformation, which rotates the odd-site spins by π angle around the z axis, both the AF and F cases give the same results. Here, we take $J>0$ for simplicity.

By applying the JW and Fourier transformations, the Hamiltonian (7) can be diagonalized as

$$H = \sum_k (J\cos k - h) c_k^\dagger c_k = \sum_k [\varepsilon(k) - h] c_k^\dagger c_k, \quad (8)$$

and the elements in the reduced density matrix [Eq. (3)] can be explicitly expressed as

$$Z_i = \frac{1}{N}\sum_k e^{ik} f(k), \quad \langle n_i\rangle = \frac{1}{N}\sum_k f(k), \quad (9)$$

$$X_i^+ = -\frac{1}{N^2}\sum_{k_1,k_2} (1 - e^{i(k_1-k_2)})\langle c_{k_1}^\dagger c_{k_2}^\dagger c_{k_1} c_{k_2}\rangle, \quad (10)$$

where $f(k)=1/[e^{\beta(\varepsilon(k)-h)}+1]$ (β is the inverse temperature and the Boltzmann constant is taken as $k_B=1$) is the Fermi distribution function. By the solution of the retarded Green's function $G_r(t)=\langle\langle c_{k_1}(t)c_{k_2}(t), c_{k_1}^\dagger c_{k_2}^\dagger\rangle\rangle (k_1\neq k_2)$ [10], the expectation value $\langle c_{k_1}^\dagger c_{k_2}^\dagger c_{k_1} c_{k_2}\rangle$ in Eq. (10) is obtained as

$$\langle c_{k_1}^\dagger c_{k_2}^\dagger c_{k_1} c_{k_2}\rangle = -f(k_1)f(k_2) \quad (k_1 \neq k_2), \quad (11)$$

and Eq. (10) is simplified as

$$X_i^+ = \langle n_i\rangle^2 - Z_i^2. \quad (12)$$

By substituting Eqs. (9) and (12) into Eq. (6), $\tilde{C}_i$ can be obtained as

$$\tilde{C}_i = -\frac{2}{\pi}\left[\int_{-1}^{1} \frac{x\,dx}{\sqrt{1-x^2}(e^{\beta'(x-h')}+1)} + \sqrt{\left(\int_{-1}^{1}\sqrt{\frac{1+x}{1-x}}\frac{dx}{e^{\beta'(x-h')}+1}\right)\left(\int_{-1}^{1}\sqrt{\frac{1-x}{1+x}}\frac{dx}{e^{\beta'(x-h')}+1}\right)} \times \sqrt{\left(\frac{1}{\pi}\int_{-1}^{1}\sqrt{\frac{1+x}{1-x}}\frac{dx}{e^{\beta'(x-h')}+1} - 1\right)\left(\frac{1}{\pi}\int_{-1}^{1}\sqrt{\frac{1-x}{1+x}}\frac{dx}{e^{\beta'(x-h')}+1} - 1\right)}\right], \quad (13)$$

where $\beta'=\beta J$ and $h'=h/J$. The result of Eq. (13) is shown in Fig. 1, where the TEs in different fields vanish at a common CT (T_c), which is a fixed point. This common CT indicates that the magnetic field cannot retrieve the intrinsic TE once it is destroyed by thermal fluctuations, even though the field changes the TE below the CT.

At $T=T_c$, $\tilde{C}_i=0$ and $Z_i^2=X_i^+X_i^-$. Thus, we can derive the equation

$$\langle n_i\rangle - \langle n_i\rangle^2 = -\sqrt{2}Z_i - Z_i^2 \quad (14)$$

at T_c for any fields. We define $\Phi(\beta,h)=\langle n_i\rangle+\sqrt{2}Z_i+Z_i^2-\langle n_i\rangle^2$, which can be expressed as

$$\Phi(\beta,h) = \frac{1}{\pi}\int_{-1}^{1} \frac{(1+\sqrt{2}x)dx}{\sqrt{1-x^2}(e^{\beta'(x-h')}+1)} + \frac{1}{\pi^2}\int_{-1}^{1}\int_{-1}^{1} \frac{(xy-1)dxdy}{\sqrt{(1-x^2)(1-y^2)}(e^{\beta'(x-h')}+1)(e^{\beta'(y-h')}+1)}. \quad (15)$$

Thus, $\Phi<0$ describes the entangled state, and Φ must be zero at T_c, i.e., $\Phi(\beta_c,h)=0$, from which T_c can be determined. In the absence of magnetic field, $\langle n_i\rangle=1/2$ at any temperatures, thus, $Z_{i,h=0}^{T_c}=(1-\sqrt{2})/2$, and T_c can be obtained by solving the equation

$$\frac{\sqrt{2}-1}{2} = \frac{J}{\pi T_c}\int_0^1 \frac{\sqrt{1-x^2}dx}{1+\cosh\frac{Jx}{T_c}}, \quad (16)$$

which indicates that T_c is proportional to J, i.e., $T_c=\alpha J$ with $\alpha\simeq 0.484\,3$. At T_c, $\Phi(\beta_c,h)$ is independent of h, i.e., $\partial\Phi(\beta_c,h)/\partial h=0$, yielding the equation

$$2(1+\sqrt{2}Z_i)\frac{\partial Z_i}{\partial h} = \sqrt{2}(2\langle n_i\rangle-1)\frac{\partial\langle n_i\rangle}{\partial h}, \quad (17)$$

which is satisfied at T_c for any fields. This equation, as well as Eq. (14), determines the fixed point completely. In Ref. [9], the CT for the $S=1/2$ two cyclic XY qubits is $0.567\,3J$, which is larger than the CT $0.484\,3J$ in the thermodynamic limit. This is consistent with the result in Ref. [8], where the CT of the spin-1/2 Heisenberg chains with $N=5\sim10$ is smaller than that with $N=2$.

In terms of the spin operators, the finite pairwise TE survives when

$$\left(\langle S_i^+S_{i+1}^-\rangle + \frac{\sqrt{2}}{2}\right)^2 < \frac{1}{4} + \langle S_i^z\rangle^2, \quad (18)$$

which indicates that the concurrence of TE is determined by the competition between the spin fluctuations and local magnetic moment at finite temperature. As the quantities in Eq. (9) can be expressed as thermodynamic observables as

$$Z_i = \frac{U+Mh}{NJ} + \frac{h}{2J}, \quad \langle n_i\rangle = \frac{M}{N} + \frac{1}{2}, \quad (19)$$

where $U=\langle H\rangle$ is the internal energy, and $M=\Sigma_i\langle S_i^z\rangle$ is the total magnetization, the TE can be witnessed by the negative thermal quantity

$$\Phi(U,M,h) = \left(\frac{U+Mh}{NJ} + \frac{h}{2J} + \frac{\sqrt{2}}{2}\right)^2 - \left(\frac{M}{N}\right)^2 - \frac{1}{4}, \quad (20)$$

which can be measured in experiment. Without the field, the magnetization M vanishes, and the TE survives when

$$\frac{|U|}{NJ} > \frac{\sqrt{2}-1}{2}, \quad (21)$$

which includes a wider parameter region than the sufficient condition $|U|/NJ>1/4$ for the entangled state that is proposed for the spin chains with Heisenberg or XY interactions [5]. In a magnetic field, Eq. (20) also implies that the witness $|U+Mh|/NJ>1/4$ proposed in Ref. [5] can be improved to cover a wider parameter region for the entangled state. The exact solution not only confirms that the CT of the intrinsic TE which survives in the absence of field is a fixed point, but also reveals some features at the fixed point from the perspectives of the local spin competition and macroscopic thermodynamic behavior.

To investigate the possible exceptions of the field independence of the CT, we study the TE in an $S=1/2$ AF-F alternating Heisenberg chain by means of the TMRG. The Hamiltonian of this alternating chain is given by

$$H = \sum_j (J_a\mathbf{S}_{2j-1}\cdot\mathbf{S}_{2j} + J_f\mathbf{S}_{2j}\cdot\mathbf{S}_{2j+1}) - h\sum_j S_j^z, \quad (22)$$

where $J_a>0$, $J_f<0$ denote the AF and F couplings, respectively. J_a is taken as the energy scale and $J_f/J_a=-1$. This AF-F chain has a Haldane gap $\Delta\simeq 0.6J_a$ in the ground state [11], and the saturation field $h_s\simeq 1.1J_a$. In experiment, this model has been realized and studied extensively [12]. The TMRG [13] method is a powerful tool for studying the thermodynamics of one-dimensional quantum systems in the thermodynamic limit [14]. In our calculations, the width of the imaginary time slice is taken as $\varepsilon=0.1$, and the error caused by the Trotter-Suzuki decomposition is less than 10^{-3}. During the TMRG iterations, 60 states are retained, and the truncation error is less than 10^{-6}.

Owing to the alternation of the couplings, the TEs of the spins coupled by J_a and J_f, which are denoted as C_a and C_f, respectively, are expected to be distinct. Figure 2(a) shows the temperature dependence of the TE C_a at different fields. It is shown that in the absence of the field, the intrinsic TE survives, and C_a vanishes at $T_c^a\simeq 0.85J_a$ due to thermal fluctuations. In the presence of the field, the CT keeps invariant. Although the alternation is involved, the CT of the intrinsic TE is still a fixed point.

However, the entanglement induced by the field does not comply to such rule. For the F couplings, the TE of the spins coupled by J_f is absent without a field. When the applied field closes the gap and increases up to about $0.9J_a$, the TE is induced by the field, as shown in Fig. 2(b). With further increasing the field, the CT of the field-induced TE enhances to reach the maximum at the saturation field. A further increase in the field makes the field-induced TE vanish as the spins are fully polarized at zero temperature. It can be seen that—different from the intrinsic TE—the CT of the field-induced TE is dependent on the magnetic field.

Furthermore, the intrinsic TE of the $S=1/2$ AF-AF-AF-F tetrameric Heisenberg chain [15] is studied using the TMRG, which are not presented here. It is shown that the CT retains a fixed point, which is also observed in the trimerized F-F-AF chain [16]. The observations suggest that the CT of

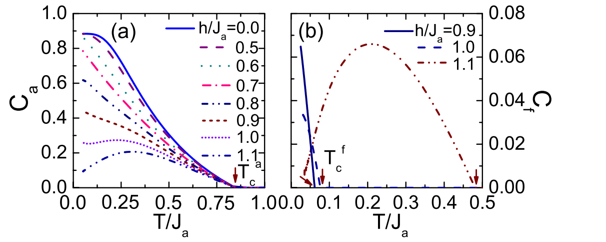

FIG. 2. (Color online) Temperature dependence of the thermal entanglement of (a) C_a and (b) C_f for the $S=1/2$ AF-F chain at various fields obtained by means of the TMRG.

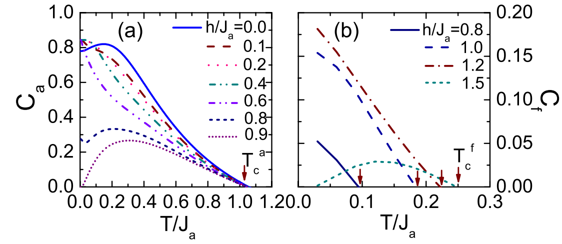

FIG. 3. (Color online) Temperature dependence of the thermal entanglement of (a) C_a and (b) C_f for the $S=1/2$ AF-F chain at various fields obtained by the mean-field theory.

the intrinsic TE in one-dimensional Heisenberg antiferromagnets might be a fixed point.

Next, we treat the AF-F chain within the mean-field framework, which may extend the discussions to the general $S=1/2$ alternating Heisenberg antiferromagnetic chains with nearest-neighbor interactions. Following the steps in Ref. [17], we make the Hartree-Fock approximation to the Hamiltonian (22) after the JW and Fourier transforms and obtain the mean-field Hamiltonian after omitting a constant,

$$H_{HF} = \sum_k \left\{ \left[(J_a + J_f)\left(d_b - \frac{1}{2}\right) - h \right] a_k^\dagger a_k + \left[(J_a + J_f)\left(d_a - \frac{1}{2}\right) - h \right] b_k^\dagger b_k \right\} + \sum_k \left[J_a\left(\frac{1}{2} - p_{ab}\right) e^{ik/2} a_k^\dagger b_k + \text{H.c.} + J_f\left(\frac{1}{2} - p_{ba}\right) e^{ik/2} b_k^\dagger a_k + \text{H.c.} \right], \quad (23)$$

where $d_a=\langle a_j^\dagger a_j\rangle$, $d_b=\langle b_j^\dagger b_j\rangle$, $p_{ab}=\langle b_j^\dagger a_j\rangle$, and $p_{ba}=\langle a_{j+1}^\dagger b_j\rangle$, which are obtained by self-consistent calculations. Then the Bogoliubov transformation is taken to diagonalize the above Hamiltonian. Thus, the TE can be calculated from the quasiparticle representation. Figure 3 shows the mean-field results of the TE C_a and C_f. It is shown that although the values of the critical fields and CT are not accurate, the mean-field results still preserve the features of the CT. The intrinsic TE C_a vanishes at a common CT, while the field-induced TE C_f is dependent on the field. As shown in Fig. 3(b), the CT of C_f enhances with increasing the field until to the maximum at the saturation field, which is analogous to the TMRG result.

In this fermion mapping $Z_{ab}=p_{ab}^*$ and $X_{ab}^+=d_a d_b - Z_{ab}^2$, where Z_{ab} and X_{ab}^+ are the values defined in Eq. (3) of the spins coupled by J_a. Thus, the concurrence C_a can be expressed by Eq. (6) using these quantities. At the CT (T_c^a), we have

$$[|p_{ab}|^2 - d_a(d_b-1)][|p_{ab}|^2 - d_a(d_b-1)] = 2|p_{ab}|^2. \quad (24)$$

The calculations show that p_{ab} is real and $d_a=d_b$. Thus, the above equation can be simplified as

$$d_a - d_a^2 = -\sqrt{2}p_{ab} - p_{ab}^2, \quad (25)$$

which has the same form as that of the XY chain [Eq. (14)], yielding the following inequality:

$$\left(\langle S_{2j-1}^+ S_{2j}^- \rangle + \frac{\sqrt{2}}{2}\right)^2 < \frac{1}{4} + \langle S_{2j-1}^z \rangle^2, \quad (26)$$

for the entangled C_a. For the field-induced TE C_f, we have $d_a - d_a^2 = -\sqrt{2}p_{ba} - p_{ba}^2$ at the CT, which is satisfied at different CTs for different fields. The entangled C_f is described by $(\langle S_{2j}^+ S_{2j+1}^- \rangle + \frac{\sqrt{2}}{2})^2 < \frac{1}{4} + \langle S_{2j}^z \rangle^2$. Note that the thermal quantity witness cannot be written in a form as simple as Eq. (20) within the present self-consistent calculations.

In summary, we have studied the field dependence of the CT of TE in the $S=1/2$ spin chains within the thermodynamic limit $N\to\infty$. The concurrence of the TE in the spin-1/2 XY chain is exactly resolved. It is found that the CT of the TE is a fixed point. An equation is given to determine the CT, which is found to be $T_c \simeq 0.484\,3J$ and smaller than that of the two-qubit system. The thermal witness for the entangled state is also proposed. Furthermore, the TE of an $S=1/2$ AF-F chain is studied by means of the TMRG method and mean-field treatment, which indicates that the CT of the intrinsic TE of the spins coupled by AF couplings is a fixed point, while that of the field-induced TE of the spins coupled by F couplings changes with the field. The exact solution of the XY chain as well as the mean-field result of the AF-F chain indicates that the disappearance of the TE is determined by the competition between the spin fluctuations and local magnetic moment at finite temperatures. The observations suggest that it may be a general phenomenon in one-dimensional Heisenberg antiferromagnets that the CT of the intrinsic TE is a fixed point independent of the magnetic field.

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