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Thermal entanglement of spin chains with quantum critical behavior

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Results for the characteristics of the macroscopic thermal entanglement for integrable spin-1/2 antiferromagnetic chain models with multispin interactions in the thermodynamic limit are presented. Such interactions cause quantum-phase transitions to incommensurate phases with partial spontaneous magnetization. We have derived exact equations, which determine the thermal and magnetic field behavior of the concurrence of spin chains. The analysis of these equations shows that there exists a critical temperature, below which the thermal entanglement of considered spin chains is nonzero. We have shown that at those quantum-phase transitions, caused by multispin interactions, the thermal entanglement is reduced. Also, we have shown that the thermal entanglement is reduced due to nonzero magnetization of spin chains in the ground state, caused by multispin interactions.

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I. INTRODUCTION

Correlation between systems contains the information of one system about another. Hence the correlation is the main issue of the many-body physics. The origin of correlations can be either classical or quantum. Very often researchers study the quantum entanglement, which describes intrinsic correlations between systems incurred in quantum mechanics. Entanglement is the fundamental aspect of the quantum many-body physics because it demonstrates the nonlocal nature of the theory, in which the entangled system contains correlations that cannot be attributed to its' subsystems alone. Macroscopic entanglement demonstrates that nonlocal correlations persist even in the thermodynamic limit. It is believed that the macroscopic entanglement has to play an essential role in the quantum information[1] (including the quantum cryptography[2]) and teleportation.[3]

In particular, many studies were devoted to the problem of the quantum entanglement in quantum spin-1/2 chain models because that class of models often permits exact solutions.[4] The characteristic feature of quantum-chain models is the possibility of quantum-phase transitions there. Quantum-phase transitions take place when the ground state of a many-body system undergoes a qualitative change by variation in some external parameter (other than the temperature).[5] Clearly, correlations, and, hence, the quantum entanglement, should be very sensitive to the fact, whether a quantum-phase transition takes place or not, and how close is the quantum critical point. Spin-1/2 chain models permit to calculate many characteristics of the entanglement, in particular, the macroscopic entanglement.

Here we present results for the thermal entanglement of several quantum spin-1/2 antiferromagnetic chains, in which quantum-phase transitions, governed by multispin interactions, take place. Obviously, it is very important to study characteristics of the entanglement for nonzero temperatures because such characteristics can be observed experimentally, unlike the ones in the ground state. The thermal entanglement for spin systems was studied recently theoretically (however, mostly for few-spin systems, not the macroscopic entanglement).[6] Moreover, several experimental groups recently reported the observation of the thermal entanglement in real magnetic systems.[7] The effect of quantum critical points on the entanglement in those investigations was studied for spin models, in which the phase transitions were caused by the external magnetic field. However, it is important to know how the internal parameters, such as additional spin-spin interactions, which are often present in real quasi-one-dimensional spin systems,[8] affect the entanglement in spin chains. The goal of our work is to determine how multispin interactions, especially ones, which cause partial spontaneous magnetization of spin chains, affect the thermal entanglement in those chains.

II. CHARACTERISTICS OF THE ENTANGLEMENT IN QUANTUM SPIN-1/2 CHAINS

The bipartite (pairwise) entanglement of two spins $S=\frac{1}{2}$ situated at the sites n and m of the quantum chain can be studied by using the reduced density matrix ρ_{nm}. The latter can be expressed, as usually, as a 4×4 matrix $\rho_{nm}=(1/4)\Sigma_{\mu,\nu}\langle\sigma_n^\mu\sigma_m^\nu\rangle\sigma_n^\mu\otimes\sigma_m^\nu$, where $\mu,\nu=0,x,y,z$ and $\sigma_m^0=I_m$, the unity matrix, $\sigma_n^\mu\otimes\sigma_m^\nu$ denotes the direct product, and brackets denote averaging in the ground state or at nonzero temperature.[9] For a homogeneous uniaxial spin chain in the absence of the Dzyaloshiskii-Moriya antisymmetric relativistic-exchange interaction one can take the advantage of the knowledge of the symmetries of the chain in the spin subspace. It implies that the reduced density matrix for that chain can be written as

$$4\rho_{nm}=\hat{I}_{nm}+\begin{pmatrix} Z+2m & 0 & 0 & 0 \\ 0 & -Z & 2X & 0 \\ 0 & 2X & -Z & 0 \\ 0 & 0 & 0 & Z-2m \end{pmatrix}, \tag{1}$$

where $\hat{I}_{nm}$ is the 4×4 unity matrix, $m=\langle\sigma_n^z\rangle$, $Z=\langle\sigma_n^z\sigma_m^z\rangle$, and $X=\langle\sigma_n^x\sigma_m^x\rangle=\langle\sigma_n^y\sigma_m^y\rangle$. Here we used the fact that the system is homogenous, $\langle\sigma_n^z\rangle=\langle\sigma_m^z\rangle$. The concurrence of the entanglement of two spins is determined as $C_{nm}=\max\{\tilde{C}_{nm},0\}$, where $\tilde{C}_{nm}=\mu_1-\mu_2-\mu_3-\mu_4$, see Ref. 10. Here $\mu_{1,2,3,4}$ (with μ_1 being the largest value) are the square roots of the eigenvalues of the matrix $\rho_{nm}\tilde{\rho}_{nm}$, where $\tilde{\rho}_{nm}$ is the spin-flipped matrix of ρ_{nm}, $\tilde{\rho}_{nm}=\sigma_n^y\otimes\sigma_m^y\otimes\rho^*\otimes\sigma_n^y\otimes\sigma_m^y$. Then the entanglement of formation is

$$E_f=-x\log_2 x-(1-x)\log_2(1-x), \tag{2}$$

where $x=(1/2)+\sqrt{1-(C_{nm}^2/2)}$. E_f is a monotonous function of the concurrence with $E_f(C_{nm}=0)=0$ and $E_f(C_{nm}=1)=1$, this is why, for simplicity we study the concurrence in what follows.

One can see that for the uniaxial spin-$\frac{1}{2}$ chain without Dzyaloshinskii-Moriya coupling the concurrence can be calculated using either the function

$$\tilde{C}_{nm}=\frac{1}{2}(\pm 2X-\sqrt{(1+Z)^2-4m^2}) \tag{3}$$

or depending on the parameters of the spin-spin interactions

$$\tilde{C}_{nm}=\frac{1}{2}(Z-1). \tag{4}$$

Obviously, at the critical temperature, below which the concurrence is positive and the thermal entanglement survives, the equalities are satisfied

$$2X_c=\pm\sqrt{(1+Z_c)^2-4m_c^2} \tag{5}$$

or

$$Z_c=1, \tag{6}$$

where the subscript c defines the value at the critical temperature. For antiferromagnetic systems one expects $X,Z<0$, hence, the last equation can be neglected.

In what follows we limit ourselves with the thermal entanglement of nearest-neighbor spins $m=n+1$ for integrable quantum-spin chains with multispin interactions. It is important to study the behavior of the macroscopic thermal entanglement in spin-1/2 chains with the SU(2)-symmetry of spin-spin interactions or for systems with the uniaxial magnetic anisotropy, which are described by the reduced density matrix Eq. (1), in which quantum critical points are present.

III. INTEGRABLE SPIN-1/2 CHAINS WITH MULTISPIN INTERACTIONS

One knows exactly solvable spin-1/2 chain models with antiferromagnetic nearest-neighbor interactions, which permit partial nonzero magnetization at $T=0$, see Refs. 11–13. The characteristic feature for those models is the presence of three-spin or four-spin interaction terms in the Hamiltonians. The nonzero partial magnetization (less than the nominal one, i.e., the ground state is not spin saturated) can take place either for the isotropic and "easy-axis" magnetically anisotropic chains[11,12] at some region of the multispin coupling parameter or for spin chains with the "easy-plane" magnetic anisotropy.[13] The phase with the nonzero ground-state magnetization is the incommensurate one.[11,12] Similar three-spin interactions were introduced later in the Kitaev spin-1/2 model on a honeycomb lattice.[14]

Let us consider the model with uniaxial spin-$\frac{1}{2}$ antiferromagnetic exchange coupling between spins and three-spin interaction, which is described by the Hamiltonian $\mathcal{H}=\mathcal{H}_0+\mathcal{H}_3$, where

$$\mathcal{H}_0=\sum_n[J(\sigma_n^x\sigma_{n+1}^x+\sigma_n^y\sigma_{n+1}^y)+J_z\sigma_n^z\sigma_{n+1}^z]-\frac{H}{2}\sum_n\sigma_n^z \tag{7}$$

and

$$\mathcal{H}_3=8J_3\sum_n(\Delta[\sigma_n^x(\sigma_{n-1}^y\sigma_{n+1}^z-\sigma_{n-1}^y\sigma_{n+1}^z)+\sigma_n^y(\sigma_{n-1}^z\sigma_{n+1}^x-\sigma_{n-1}^x\sigma_{n+1}^z)]+\sigma_n^z(\sigma_{n-1}^x\sigma_{n+1}^y-\sigma_{n-1}^y\sigma_{n+1}^x)), \tag{8}$$

where $\Delta=J_z/J$. The model is exactly solvable for any values of the coupling constants J, J_z, and J_3, and the external magnetic field H. Here we limit ourselves with $J,J_z>0$, and periodic boundary conditions. In our study we use the units in which the Boltzmann's constant, the effective g factor, and the Bohr's magneton are equal to unity. Let us define $\Delta=\cosh\eta$. The critical situation with the easy-plane magnetic anisotropy is described, as usually, by the change $\eta=-i\gamma$.

Uniaxial one-dimensional spin-1/2 models are known to have no magnetic ordering even in the ground state,[4] except of the trivial one, at $H>H_s$, $H_s=J+J_z$, where such spin systems are in the ferromagnetic spin-polarized state. The entanglement in such a state is, obviously, zero, because the eigenfunction of the state of the multispin system is the product of the eigenfunctions of eigenfunctions of each spin. By the way, it is the reason, why we do not consider here the ferromagnetic spin-1/2 chains: for them we expect either zero entanglement (in the spin-polarized ground state) or a small one for a state with nonzero temperatures.

However, it is interesting to find how quantum critical points and partial spontaneous magnetization can affect the behavior of a critical temperature for the macroscopic entanglement in spin chains. One known example is the spin-1/2 Ising chain in the transverse field.[15] However, in that model one deals with the case of extremely large biaxial magnetic anisotropy of spin-spin interactions. There is no spontaneous magnetization in that model and the quantum critical point there is not governed by the internal parameter (such as additional spin-spin interactions) but by the external magnetic field.

The incommensurate phase for the uniaxial antiferromagnetic spin-1/2 chain model with the Hamiltonian Eqs. (7) and (8) takes place at $J_3>J_3^{(c)}=4\gamma J/\pi\sin\gamma$ for positive J_3 and $0<\Delta<1$, i.e., for the easy-plane antiferromagnetic case.[11,12] For the easy-axis anisotropy of the antiferromagnetic chain the critical value is $J_3^{(c)}=2\eta J/kK'(k)\sinh\eta$, where $\eta=\pi K'(k)/K(k)$, $K(k)$ and $K'(k)$ are the complete elliptic integrals of the first kind with modulus k and $k'=\sqrt{1-k^2}$, respectively.[11] The phase diagram of the model as a function of the external magnetic field and the multispin interaction is

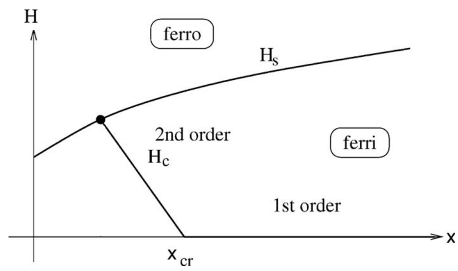

FIG. 1. The phase diagram of the model as the function of the external field H and the multispin interaction $x=J_3/J$.

presented in Fig. 1 for $0<\Delta\leq 0$. If the value of the external field is larger than H_s (at which the second-order quantum-phase transition takes place), the model is in the spin-saturated (ferromagnetic) phase. As for the dependence on $x=J_3/J$: there is a critical value $x_c=J_3^{(c)}/J$, above which the model is in the incommensurate phase with the weak spontaneous magnetization (less than the nominal one) for $\Delta=1$. In that situation the line $x>x_c$ is the line of the first-order quantum-phase transition. At the critical field H_c the second-order quantum-phase transition takes place between the commensurate phase (for small fields and J_3) and the incommensurate one.[11,12]

We will also study the important particular case $J_z=\Delta=0$ (known as the isotropic XY model). In that case the model with the Hamiltonian $\mathcal{H}$ is also exactly solvable but is does not reveal the spontaneous magnetization in the ground state. This is why, in this work we will also study the model[13] with the Hamiltonian $\mathcal{H}^{(1)}=\mathcal{H}_0(J_z=0)+\mathcal{H}_3^{(1)}$, where

$$\mathcal{H}_3^{(1)} = 8J_3^{(1)}\sum_n \sigma_n^z(\sigma_{n-1}^x\sigma_{n+1}^x + \sigma_{n-1}^y\sigma_{n+1}^y). \qquad (9)$$

It is known that for such a model three-spin interactions also cause partial spontaneous magnetization in the ground state.

IV. THERMAL ENTANGLEMENT FOR CONSIDERED MODELS

The temperature and magnetic field dependencies of the correlation functions X, Z, and (twice) the magnetization m of the spin-$\frac{1}{2}$ chain with the Hamiltonian $\mathcal{H}$ can be written in the thermodynamic limit as (those exact results are obtained in the framework of the thermal Bethe's ansatz, or the "quantum-transfer matrix" approach, cf. Ref. 16)

$$Z = A\Delta + B,$$

$$2X = -A - B\Delta,$$

$$m = -1 - \int_{\mathcal{C}} \frac{dx}{i\pi[1+a(x)]} G(x), \qquad (10)$$

where

$$A = \frac{\Delta}{\Delta^2-1} - \int_{\mathcal{C}} \frac{dx}{i\pi[1+a(x)]} \times \frac{G(x)}{\sinh(x)\sinh(x-\eta)},$$

$$B = \frac{1}{\Delta^2-1} - \int_{\mathcal{C}} \frac{dx}{i\pi[1+a(x)]} \times \left[\frac{G''(x)\sinh(\eta)}{\eta\sinh(x)\sinh(x-\eta)} - G'(x)\coth(x-\eta)\right]. \qquad (11)$$

Functions $G(x)$, $G'(x)$, and $G''(x)$ satisfy linear integral equations

$$G(x) = \frac{\sinh(\eta)}{\sinh(x)\sinh(x-\eta)} + \int_{\mathcal{C}} \frac{dy}{i\pi[1+a(y)]} \times \frac{\sinh(\eta)\Delta G(y)}{\sinh(x-y-\eta)\sinh(x-y+\eta)},$$

$$G'(x) = \frac{1}{\sinh^2(x-\eta)} - \frac{1}{\sinh^2(x)} + \int_{\mathcal{C}} \frac{dy}{i\pi[1+a(y)]} \times \frac{G'(y)\Delta\sinh(\eta)}{\sinh(x-y-\eta)\sinh(x-y+\eta)},$$

$$G''(x) = \frac{\eta}{\sinh^2(x-\eta)} - \frac{1}{\sinh^2(x)} + \int_{\mathcal{C}} \frac{dy}{i2\pi[1+a(y)]} \times \frac{2\Delta\sinh(\eta)G''(y) + \eta\sinh(2x-2y)G'(y)}{\sinh(x-y-\eta)\sinh(x-y+\eta)}. \qquad (12)$$

The function $a(x)$ is determined from the solution of the nonlinear integral equation

$$\ln a(x) = -\frac{H}{T} + \frac{2J\sinh^2(\eta)}{T\sinh(x)\sinh(x+\eta)]} - \frac{4J_3\sinh^3(\eta)\sinh(2x+\eta)}{T\eta\sinh^2(x)\sinh^2(x+\eta)} - \int_{\mathcal{C}} \frac{dy}{i2\pi} \frac{\sinh(2\eta)\ln[1+a(y)]}{\sinh(x-y+\eta)\sinh(x-y-\eta)}, \qquad (13)$$

where T is the temperature. The contour $\mathcal{C}$ encloses the real axis at the distance $|\epsilon|<\eta/2$ for $-1\leq\Delta\leq 1$ or it encloses the imaginary axis at the distance $|\epsilon|<\eta/2$ for $\Delta>1$, in the counterclockwise manner.

In Fig. 2 we present the behavior of the concurrence of the considered model for $J_z=0$ for the case of weak enough three-spin coupling, $x=J_3/J=1.2$. The concurrence is zero at small temperatures then it becomes larger at intermediate temperatures, and, finally, at high temperatures, larger than the exchange constant, the concurrence is zero. The concurrence is not a strong function of the external magnetic field for small enough values of J_s: the temperature, at which the concurrence becomes nonzero, depends on the value of the external field weakly (however, the value of the concurrence at intermediate temperatures does depend on the magnetic

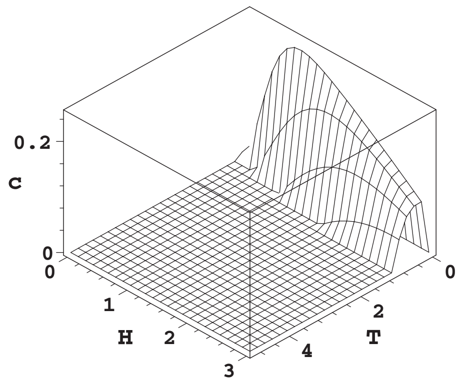

FIG. 2. The concurrence of the considered model as a function of temperature and magnetic field for $J=1$, $\Delta=0$, and $J_3=1.2$.

field). At larger values of the multispin interaction, the critical value of the temperature, at which the concurrence becomes zero, depends on the external magnetic field stronger, see Fig. 2 Our analysis shows that for this case there exists a critical value of the multispin coupling $J_3 \approx 1.242J$, above which the concurrence of the system becomes zero.

The limit of the spin chain with interactions only between two neighboring spins, $J_3=0$, is considered in detail in Appendix. Unfortunately, it is impossible to obtain analytic results for the model with $\Delta \neq 0$ for the incommensurate phase with the nonzero spontaneous magnetization. However, we can estimate how the critical temperature changes in the commensurate phase, for $J_3 < J_3^{(c)}$. In this case for $H=0$ we have $m=0$. The solution of Eq. (13) can be obtained analytically at low temperatures, cf. Refs. 4 and 17. It yields for correlation functions in the isotropic case at $H=0$

$$X = Z \approx \frac{1}{3}\left[1 - 4\ln 2 + \frac{T^2}{12J^2(1-\alpha^2)}\right], \tag{14}$$

where $\alpha = J_3/J_3^{(c)}$. The concurrence in this case is equal to $\tilde{C}_{n,n+1} = \pm X - (1/2)(1+X)$. At the critical temperature the concurrence is zero, i.e., $2X_c = \pm(1+X_c)$. It yields the estimation for the critical temperature, below which the thermal entanglement is nonzero, $T_c \approx 2J\sqrt{1-\alpha^2}\sqrt{12\ln 2 - 6} \sim 3.04J\sqrt{1-\alpha^2}$. Hence, when the system becomes closer to the quantum critical point $\alpha=1$, the critical temperature, above which the thermal entanglement is zero, becomes smaller. At the critical point one has to take into account higher order in T corrections. We can suppose, following Ref. 18, that in the incommensurate phase the temperature region, in which the thermal pairwise entanglement is nonzero, also becomes smaller, comparing to the standard spin chain with interactions only between nearest neighbor two spins (cf. Appendix), when one approaches the quantum critical point, caused by multispin interactions. Also, it turns out that the magnetic easy-plane anisotropy reduces the critical temperature, below which the thermal entanglement becomes nonzero. Notice that the obtained dependence on α is model dependent[12] while the conclusion about the reduction in the critical temperature near considered quantum critical points seems to be generic.

For $J_3=\alpha=0$ the numerical study[19] of integral equations for correlation functions X and Z implies the following. At $H=0$ the numerical solution states that the nearest-neighbor correlation functions are temperature dependent in a narrow temperature region near $T \sim J$ for all values of the magnetic anisotropy. For $T \gg J$ for all $\Delta > 0$ both X and Z are zero in the absence of the external magnetic field. At $H=0$, for $T \ll J$, X and Z are approximately constants (for the isotropic case they are ~ -0.6), and the values for Z become larger for smaller Δ (for the XY chain it is ~ -0.4), while for X the values become a little smaller for smaller Δ. Hence, numerical solutions for correlation functions qualitatively agree with our analytical low-temperature asymptotics, supporting our estimates for the critical temperature for the thermal entanglement.

On the other hand, for the XY model with three-spin interactions with the Hamiltonian $\mathcal{H}^{(1)}$, we can calculate the concurrence exactly, as for the absence of multispin interactions, see Appendix. The critical temperature, above which the concurrence becomes zero, is determined by Eq. (A10), where

$$m = \frac{1}{\pi}\int_0^{\pi} dk\left[1 - \tanh\left(\frac{\varepsilon_k}{2T}\right)\right] - 1,$$

$$X = -\frac{1}{\pi}\int_0^{\pi} dk \cos k\left[1 - \tanh\left(\frac{\varepsilon_k}{2T}\right)\right] \tag{15}$$

and

$$\varepsilon_k = H + 2J_3^{(1)} - 4J\cos k - J_3^{(1)}\cos^2 k. \tag{16}$$

At $H=0$ the magnetization is different from zero due to $J_3^{(1)} \neq 0$. The critical temperature is determined from the equation

$$\left(\frac{1}{\pi}\right)^2 \int_0^{\pi} dk(1-\cos k)\left[1 - \tanh\left(\frac{\varepsilon_k}{2T_c}\right)\right] \times \int_0^{\pi} dk(1+\cos k)\left[1 - \tanh\left(\frac{\varepsilon_k}{2T_c}\right)\right] - \frac{2}{\pi}\int_0^{\pi} dk \times (1 - 2\sqrt{2}\cos k)\left[1 - \tanh\left(\frac{\varepsilon_k}{2T_c}\right)\right] = 0. \tag{17}$$

This equation can be solved graphically. In Fig. 3 we show the right-hand sides of Eq. (17) for several values of $J_3^{(1)}$. In fact, the curves in Fig. 3 are $-\tilde{C}_{n,n+1}$ for the studied model. One can see that the three-spin interaction reduces the critical temperature also for the XY chain. We also see that there exists the critical value of $J_3^{(1)} \approx 2.23J$, above which the macroscopic thermal entanglement is zero for any temperatures. It is determined from the equation

$$(X_c + \sqrt{2})\frac{\partial X_c}{\partial J_3^{(1)}} = m_c \frac{\partial m_c}{\partial J_3^{(1)}}, \tag{18}$$

where

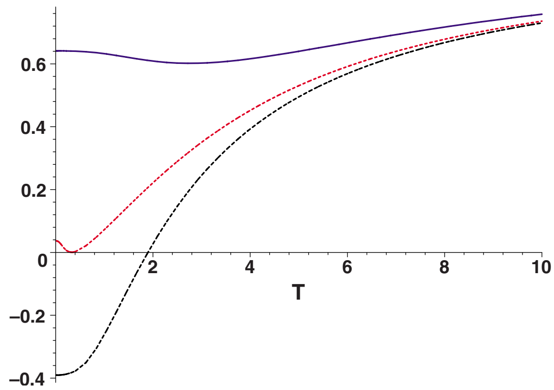

FIG. 3. (Color online) The right-hand side of Eq. (17) as a function of temperature (in the units of J) for the XY chain with three-spin interactions, which produce a spontaneous magnetization. The (black) dashed curve describes $J_3^{(1)}=0.5J$; the (red) dotted curve describes $J_3^{(1)}=2.23J$, and the (blue) solid curve is for the case with $J_3^{(1)}=5J$. The concurrence becomes zero at temperatures, higher than the crossing points of curves with the temperature axis.

$$\frac{\partial X_c}{\partial J_3^{(1)}} = \frac{2}{\pi}\int_0^{\pi} dk \cos k \frac{1+4\sin k \cos k}{\cosh^2(\varepsilon_k/2T_c)},$$

$$\frac{\partial m_c}{\partial J_3^{(1)}} = -\frac{1}{\pi}\int_0^{\pi} dk \frac{1+4\sin k \cos k}{\cosh^2(\varepsilon_k/2T_c)}. \tag{19}$$

For the experimental determination of the thermal entanglement in real quasi-one-dimensional quantum-spin systems we can suppose the following. The critical temperature, below which the thermal entanglement becomes nonzero, is determined by the behavior of pairwise spin-spin nearest-neighbor correlation functions. This is why, we may assume that the thermal entanglement for real quasi-one-dimensional spin systems is nonzero below the temperature, at which the magnetic specific heat (which is also determined by the temperature behavior of neighboring spin-spin correlation functions) has the maximum in its temperature behavior (at $H=0$).[20] Notice, that the maximum in the temperature behavior of the magnetic susceptibility can be determined simpler than the one in the temperature behavior of the magnetic specific heat and they are situated approximately at similar temperatures.[20] Observe, however, that the magnetic susceptibility is determined by spin-spin correlations from all pairs of spins (not only nearest-neighbor interactions) cf. Ref. 7.

V. SUMMARY

In summary, we have calculated the characteristics of the macroscopic thermal entanglement for several exactly solvable models of spin-1/2 antiferromagnetic chains with multispin interactions. We show that the thermal entanglement is nonzero at the temperatures, lower than the critical one, which is model dependent. The critical temperature, below which the thermal entanglement is nonzero, is maximal for the SU(2)-symmetric spin chain, and it becomes smaller for antiferromagnetic spin chains with the uniaxial magnetic anisotropy. We have found the characteristics of the thermal entanglement for spin chains with multispin interactions, which produce quantum-phase transitions to incommensurate phases. Our results clearly indicate that the thermal entanglement (and, therefore, the critical temperature) become smaller near the quantum critical point, caused by multispin interactions. Also, the partial spontaneous magnetization of states, caused by the multispin interactions, reduces the thermal entanglement and the temperature of the transition to the entangled state. This phenomenon is similar to the reduction in the entanglement for spin chains due to the external magnetic field in uniaxial spin chains, i.e., the entanglement seems to be reduced with the growth of the magnetization of the magnetically uniaxial system. It is interesting to check, whether this rule is fulfilled for other spin chains and for higher-dimensional quantum-spin models.

ACKNOWLEDGMENT

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APPENDIX

In this Appendix we consider the particular case of the model with the Hamiltonian $\mathcal{H}$ without three-spin couplings, $J_3=0$. Notice that the ground-state behavior of the entanglement of this particular case was studied in Refs. 21 and 22. The internal energy per site U is equal to

$$U = J(2X+\Delta Z) - \frac{mH}{2}$$
$$= \frac{H}{2} + J\Delta + \int_C \frac{dxG(x)}{i\pi[1+a(x)]}\left[\frac{H}{2} - \frac{J(\Delta^2-1)}{\sinh(x)\sinh(x-\eta)}\right]. \tag{A1}$$

In the absence of the magnetic field, $H=0$, we have, naturally, $m=0$ for any temperatures and exchange constants.

Let us study the most important cases $J_z=J$ (i.e., the isotropic Heisenberg spin-$\frac{1}{2}$ antiferromagnetic chain, in which, according to Ref. 21, the largest concurrence for any uniaxial homogeneous spin-1/2 chain with nearest-neighbor interactions takes place) and $J_z=0$ (i.e., the isotropic XY model).

In the first case, $\eta \to 0$, the formulas can be rewritten in a convenient way as $Z=-(a/3)+(2b/3)$ and $2X=-(2a/3)-(2b/3)$, where

$$a = \int_C \frac{d\omega}{\pi[1+a(\omega)]}\frac{G(\omega)}{\omega(\omega-i)} - 1 \tag{A2}$$

and

$$b = \left[\int_C \frac{d\omega}{\pi[1+a(\omega)]}G(\omega) - 1\right]$$
$$\times \left[\int_C \frac{d\omega}{\pi[1+a(\omega)]}\omega G'(\omega) - 1\right] - \int_C \frac{d\omega}{\pi[1+a(\omega)]}G'(\omega)$$
$$\times \left[\int_C \frac{d\omega}{\pi[1+a(\omega)]}\omega G(\omega) - \frac{i}{2}\right], \tag{A3}$$

where $G(\omega)$ and $G'(\omega)$ satisfy linear integral equations

$$G(\omega) + \frac{1}{\omega(\omega - i)} = \int_C \frac{d\lambda}{\pi[1 + a(\lambda)]} \frac{G(\lambda)}{1 + (\omega - \lambda)^2},$$

$$G'(\omega) + \frac{i}{\omega^2(\omega - i)^2} = \int_C \frac{d\lambda}{\pi[1 + a(\lambda)]} \frac{G'(\lambda)}{1 + (\omega - \lambda)^2} \tag{A4}$$

and $a(\omega)$ follows from the nonlinear integral equation

$$\ln a(\omega) = -\frac{H}{T} + \frac{2J}{T\omega(\omega + i)} - \int_C \frac{d\lambda}{\pi} \frac{\ln[1 + a(\lambda)]}{1 + (\omega - \lambda)^2}. \tag{A5}$$

At $H=0$ we have $m=0$ and $b=0$, $X=Z=-(a/3)$. The internal energy per site is $U=J(2X+Z)=-Ja$.

Unfortunately, it is possible to obtain solutions to the integral equations for any temperatures only numerically. However, at low temperatures it is possible to obtain analytical results. The low-temperature solution at $H=0$ to these equations yields, cf. Refs. 4, 17, and 23

$$a \approx -1 + 4 \ln 2 - \frac{T^2}{12J^2}\left[1 + \frac{3}{8}\frac{1}{\ln^3(aJ/T)} + \ldots\right] + O(T^4), \tag{A6}$$

where $a=4\sqrt{\pi/2}\exp[\gamma+(1/4)]J \approx 11.364J$ (γ is the Euler constant, do not confuse with the parameter of the anisotropy), from which it follows that (we neglect here logarithmic corrections)

$$X = Z \approx \frac{1}{3}\left[1 - 4 \ln 2 + \frac{T^2}{12J^2}\right]. \tag{A7}$$

Then, from the equation for the critical temperature for the concurrence, we obtain the estimation for $T_c \approx 2J\sqrt{12 \ln 2 - 6} \approx 3.04484J$ in the low-temperature approximation. It implies that for $T < T_c$ the state of the Heisenberg antiferromagnetic chain at $H=0$ is entangled.

The other limiting case, $J_z=0$, corresponds to the absence of interaction (i.e., the integral equations in this limit are just usual equations). Using the exact solutions of these equations we obtain for the correlation functions

$$Z = -X^2 + m^2 - 4m + 1, \tag{A8}$$

where

$$X = -\frac{1}{\pi}\int_0^\pi dk \cos k\left[1 - \tanh\left(\frac{H - 4J\cos k}{2T}\right)\right],$$

$$m = \frac{1}{\pi}\int_0^\pi dk\left[1 - \tanh\left(\frac{H - 4J\cos k}{2T}\right)\right] - 1. \tag{A9}$$

At the critical temperature we have $X_c^2=(1/4)(1+Z_c)^2-m^2$, which implies

$$X_c^2 + 2\sqrt{2}X_c + 1 - m_c^2 = 0. \tag{A10}$$

In the absence of the magnetic field we have $m=0$, and, hence, $X_c=-\sqrt{2}+1$. We can also estimate the critical temperature using the low-temperature asymptotics. The low-temperature approximation for the determination of T_c, which we used for the determination of the critical temperature, gives

$$4(1 - \sqrt{2}) = -\frac{8}{\pi} + \frac{\pi T_c^2}{24J^2}. \tag{A11}$$

The solution of this equation yields $T_c \approx 2.6069J$.

On the other hand, for the *XY* model we can find the critical temperature exactly. The critical temperature for $H=0$ is determined from the equation

$$\sqrt{2} - 1 = \frac{1}{\pi}\int_0^\pi dk \cos k\left[1 + \tanh\left(\frac{2J\cos k}{T_c}\right)\right]. \tag{A12}$$

The calculations yield the result $T_c \approx 1.9372J$. It implies that the low-temperature approximation, used above for the Heisenberg antiferromagnetic spin chain, also gave a little overestimated value for the critical temperature.

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