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Correlation entropy and the Kosterlitz–Thouless transition

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Abstract
A relation between the correlation entropy and the correlation functions for the general spin-$1/2$ systems is obtained. It is shown that the correlation entropy catches some characters of correlation behavior and can be used to quantify the quantum and finite-temperature phase transitions, including the infinite order or topological ones. As an example, the Kosterlitz–Thouless transition in the quantum two-dimensional XY model is investigated. The critical temperature and the critical exponents are determined from the finite-size scaling analysis of the correlation entropy.

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1. Introduction

The interdisciplinary fields in condensed matter physics, quantum information and quantum computation show many attractive phenomena. For example, quantum entanglement, as one of the most fundamental concepts in quantum information theory, has been used to quantify the phase transitions in condensed matter systems [1–12]. Osterloh *et al* [1] and Osborne *et al* [2] found that the concurrence or its derivative of two sites with their nearest neighbor shows a peak near or at the critical point, which can be used to identify the quantum phase transition in spin systems. Gu *et al* [3] studied the local entanglement of single sites in a fermionic system and found that the critical point corresponds to the maximum point of the entanglement. Cao *et al* [4] showed that the partial entropy, which is the classical counterpart of von Neumann entropy, has finite-size scaling behavior near the critical temperature and it can be used to quantify the finite-temperature phase transitions in both the classical and the quantum systems.

The Kosterlitz–Thouless (KT) transition [13, 14] is an important issue in the modern theory of critical phenomena. This phase transition is an infinite order or topological one and exists in some interacting spin systems such as the 2D XY model. The 2D XY model possesses the $U(1)$ symmetry and a finite-temperature phase transition, but the expected second-order one is destroyed by the transverse fluctuations. If the temperature is lower than the critical temperature, the system has a phase with a power-law correlation. While if the temperature is higher than the critical point, the system has a phase with the exponential correlation. The 2D XY model can be physically realized in a 2D Josephson junction and has been extensively studied [15–18]. For example, Doniach studied the quantum fluctuation in 2D Josephson junction array [15]. By using the Monte Carlo method, Jacobs *et al* studied the coherence states in the periodic arrays of ultrasmall Josephson junction [16]. In terms of real space renormalization group of topological excitations in the system, Williams [17], and Chattopadhyay and Shenoy [18] found a 3D vortex-loop description of the KT transition.

To the KT transition, most of the entanglement measurements such as concurrence, local entanglement and partial entropy are failed to describe. A good entanglement measurement should catch the most essential feature of the phase transitions, i.e., the correlation behavior near the critical point. In this paper, we study the correlation effects from the view of entropy. We find that the correlation entropy catches some intrinsic characters of the phase transitions and can be used to determine the critical points. Comparing with the correlation function, the correlation entropy method has many advantages. For example, the correlation entropy includes all kinds of correlation effects, the correlation entropy shows the finite-size scaling behavior for the small systems, and it does not need the pre-assumed order parameter.

In this work, we give a relation between the correlation entropy and the correlation functions in the general spin-1/2 systems. Then, we derive the finite-size scaling law of the correlation entropy. By using the stochastic series expansion (SSE) quantum Monte Carlo (QMC) simulation with operator-loop update [19–21], we study the KT transition in quantum 2D XY model. From the finite-size scaling analysis of the correlation entropy, we obtain the critical temperature and the critical exponents. Our results agree with the pervious ones.

The paper is organized as follows. In section 2, we derive the correlation entropy and its the finite-size scaling law. In section 3, we show that the correlation entropy can be used to quantify the KT transition. Section 4 is the summary.

2. Correlation entropy

In a many-body system, there exists interactions among the subsystems and the states of subsystems are entangled with each other. The correlation functions are used to quantify the correlation effects. Another important concept, correlation entropy, are suggested to quantify the correlation effects from the entropy point of view [22–25]. The correlation entropy is defined as

$$S(A:B) = S_A + S_B - S_{AB}, \tag{1}$$

where A and B are two subsystems in the real physical system, $S_p = -\mathrm{tr}(\rho_p \log_2 \rho_p)$ is the partial entropy of subsystem $p = A, B$, $\rho_p = \mathrm{tr}_{\bar{p}}\rho$ is the reduced density matrix of subsystem p, $\mathrm{tr}_{\bar{p}}$ stands for tracing over all except the selected subsystem p and ρ is the density matrix of the system. The correlation entropy measures the correlation intensity between two subsystems. In the information theory, the correlation entropy is called the mutual information [26, 27], which is a measure of quantum entanglement [28–30].

For a spin-1/2 system, the general form of single-site reduced density matrix is

$$\rho_i = \tfrac{1}{2}\left(I + \langle\sigma_i^x\rangle\sigma_i^x + \langle\sigma_i^y\rangle\sigma_i^y + \langle\sigma_i^z\rangle\sigma_i^z\right), \tag{2}$$

where I is the identity matrix and $\sigma_i^\alpha(\alpha = x, y, z)$ are the Pauli matrices at the site i. From the eigen equation

$$\begin{vmatrix} \lambda - \frac{1}{2}\left(1+\langle\sigma_i^z\rangle\right) & \frac{1}{2}\left(\mathrm{i}\langle\sigma_i^y\rangle - \langle\sigma_i^x\rangle\right) \\ -\frac{1}{2}\left(\mathrm{i}\langle\sigma_i^y\rangle + \langle\sigma_i^x\rangle\right) & \lambda - \frac{1}{2}\left(1-\langle\sigma_i^z\rangle\right) \end{vmatrix} = 0, \tag{3}$$

we obtain the eigenvalues of the reduced density matrix (2) as $\lambda_{1,2} = (1 \pm r)/2$, where $r = \left(\langle\sigma_i^x\rangle^2 + \langle\sigma_i^y\rangle^2 + \langle\sigma_i^z\rangle^2\right)^{1/2}$. The partial entropy of subsystem i is $S_i = -\sum_{n=1}^{2} \lambda_n \log_2 \lambda_n$, which can also be written as

$$S_i = 1 - \frac{1}{2\ln 2}(1+r)\ln(1+r) - \frac{1}{2\ln 2}(1-r)\ln(1-r). \tag{4}$$

The quantity S_i measures the correlation between the subsystem i and the rest of the system. Using the relation of power-series expansion, $\ln(1+x) = x - x^2/2 + \cdots + (-1)^{n+1}x^n/n + \ldots, -1 < x \leqslant 1$, we have

$$\begin{aligned} S_i &= 1 - \frac{1}{\ln 2}\sum_{n=1}^{\infty}\frac{r^{2n}}{(2n-1)2n} \\ &= 1 - \frac{1}{2\ln 2}\sum_{\alpha=x,y,z}\langle\sigma_i^\alpha\rangle^2 - \frac{1}{12\ln 2}\left(\sum_{\alpha=x,y,z}\langle\sigma_i^\alpha\rangle^2\right)^2 + o(\langle\cdots\rangle^6), \end{aligned} \tag{5}$$

where $o(\langle\cdots\rangle^6)$ represents the correlation functions with terms of powers larger than or equal to the sixth order. The odd-power terms do not appear in equation (5).

The general form of two-site reduced density matrix ρ_{ij} for a spin-1/2 system is

$$\rho_{ij} = \frac{1}{4}I + \frac{1}{4}\sum_{\alpha;l=i,j}\langle\sigma_l^\alpha\rangle\sigma_l^\alpha + \frac{1}{4}\sum_{\alpha\beta}\langle\sigma_i^\alpha\sigma_j^\beta\rangle\sigma_i^\alpha\sigma_j^\beta, \tag{6}$$

which is a 4×4 matrix. The elements of reduced density matrix (6) are

$$\begin{aligned}
a_{11} &= \tfrac{1}{4}\left(1 + \langle\sigma_i^z\sigma_j^z\rangle + \langle\sigma_i^z\rangle + \langle\sigma_j^z\rangle\right), \\
a_{22} &= \tfrac{1}{4}\left(1 + \langle\sigma_i^z\rangle - \langle\sigma_j^z\rangle - \langle\sigma_i^z\sigma_j^z\rangle\right), \\
a_{33} &= \tfrac{1}{4}\left(1 - \langle\sigma_i^z\rangle + \langle\sigma_j^z\rangle - \langle\sigma_i^z\sigma_j^z\rangle\right), \\
a_{44} &= \tfrac{1}{4}\left(1 + \langle\sigma_i^z\sigma_j^z\rangle - \langle\sigma_i^z\rangle - \langle\sigma_j^z\rangle\right), \\
a_{12} &= \tfrac{1}{4}\left[\langle\sigma_j^x\rangle + \langle\sigma_i^z\sigma_j^x\rangle - \mathrm{i}\left(\langle\sigma_j^y\rangle + \langle\sigma_i^z\sigma_j^y\rangle\right)\right], \\
a_{13} &= \tfrac{1}{4}\left[\langle\sigma_i^x\rangle + \langle\sigma_i^x\sigma_j^z\rangle - \mathrm{i}\left(\langle\sigma_i^y\rangle + \langle\sigma_i^y\sigma_j^z\rangle\right)\right], \\
a_{14} &= \tfrac{1}{4}\left[\langle\sigma_i^x\sigma_j^x\rangle - \langle\sigma_i^y\sigma_j^y\rangle - \mathrm{i}\left(\langle\sigma_i^x\sigma_j^y\rangle + \langle\sigma_i^y\sigma_j^x\rangle\right)\right], \\
a_{23} &= \tfrac{1}{4}\left[\langle\sigma_i^x\sigma_j^x\rangle + \langle\sigma_i^y\sigma_j^y\rangle + \mathrm{i}\left(\langle\sigma_i^x\sigma_j^y\rangle - \langle\sigma_i^y\sigma_j^x\rangle\right)\right], \\
a_{24} &= \tfrac{1}{4}\left[\langle\sigma_i^x\rangle - \langle\sigma_i^x\sigma_j^z\rangle - \mathrm{i}\left(\langle\sigma_i^y\rangle - \langle\sigma_i^y\sigma_j^z\rangle\right)\right], \\
a_{34} &= \tfrac{1}{4}\left[\langle\sigma_j^x\rangle - \langle\sigma_i^z\sigma_j^x\rangle - \mathrm{i}\left(\langle\sigma_j^y\rangle - \langle\sigma_i^z\sigma_j^y\rangle\right)\right], \\
a_{21} &= a_{12}^*, \qquad a_{31} = a_{13}^*, \qquad a_{41} = a_{14}^*, \\
a_{32} &= a_{23}^*, \qquad a_{42} = a_{24}^*, \qquad a_{43} = a_{34}^*.
\end{aligned} \tag{7}$$

The eigenvalues of the reduced density matrix (6) should satisfy the eigen equation

$$|\lambda\delta_{mn} - a_{mn}| = 0, \tag{8}$$

which can be simplified as

$$\lambda^4 + a_3\lambda^3 + a_2\lambda^2 + a_1\lambda + a_0 = 0, \tag{9}$$

where $a_{0,1,2,3}$ are the coefficients and determined by equation (8). The partial entropy of two-site subsystem is

$$
\begin{aligned}
S_{ij} &= -\sum_{n=1}^{4} \lambda_n \log_2 \lambda_n \\
&= 2 - \frac{1}{8\ln 2} \sum_{n=1}^{4} \left[(1-4\lambda_n)^2 + \frac{1}{3}(1-4\lambda_n)^3 + o((1-4\lambda_n)^4) \right].
\end{aligned} \tag{10}
$$

From the relations between the coefficients and the roots of equation (9),

$$
a_1 = -\sum_{n\neq m\neq l} \lambda_n\lambda_m\lambda_l, \qquad a_2 = \sum_{n\neq m} \lambda_n\lambda_m, \qquad a_3 = -\sum_{n} \lambda_n, \tag{11}
$$

we have

$$
\begin{aligned}
\sum_n (1-4\lambda_n)^2 &= 16a_3^2 - 32a_2 + 8a_3 + 4, \\
\sum_n (1-4\lambda_n)^3 &= 64a_3^3 + 48a_3^2 - 192a_2a_3 + 12a_3 - 96a_2 + 192a_1 + 4.
\end{aligned} \tag{12}
$$

Considering the fact that the trace of density matrix is 1, we have $\sum_n \lambda_n = 1$. From the eigen equation (8), we obtain

$$
\begin{aligned}
a_1 &= -\frac{1}{16}\Bigg[1 - \sum_{\alpha,l} \langle\sigma_l^\alpha\rangle^2 - \sum_{\alpha\beta} \langle\sigma_i^\alpha\sigma_j^\beta\rangle^2 + 2\sum_{\alpha\beta} \langle\sigma_i^\alpha\rangle\langle\sigma_j^\beta\rangle\langle\sigma_i^\alpha\sigma_j^\beta\rangle \\
&\quad + \sum_{\alpha\neq\beta\neq\gamma} \bigg(\langle\sigma_i^\alpha\sigma_j^\alpha\rangle\langle\sigma_i^\beta\sigma_j^\gamma\rangle\langle\sigma_i^\gamma\sigma_j^\beta\rangle - \frac{2}{3}\langle\sigma_i^\alpha\sigma_j^\beta\rangle\langle\sigma_i^\beta\sigma_j^\gamma\rangle\langle\sigma_i^\gamma\sigma_j^\alpha\rangle \\
&\quad - \frac{1}{3}\langle\sigma_i^\alpha\sigma_j^\alpha\rangle\langle\sigma_i^\beta\sigma_j^\beta\rangle\langle\sigma_i^\gamma\sigma_j^\gamma\rangle \bigg) \Bigg], \\
a_2 &= \frac{1}{16}\left[6 - 2\sum_{\alpha;l=i,j} \langle\sigma_l^\alpha\rangle^2 - 2\sum_{\alpha\beta} \langle\sigma_i^\alpha\sigma_j^\beta\rangle^2 \right], \\
a_3 &= -1,
\end{aligned} \tag{13}
$$

where $\alpha, \beta = x, y, z$ and $l = i, j$.

From equations (5), (10), (12) and (13), we obtain the correlation entropy between two sites i and j as

$$
\begin{aligned}
S(i:j) &= \frac{1}{2\ln 2}\sum_{\alpha\beta} \langle\sigma_i^\alpha\sigma_j^\beta\rangle^2 - \frac{1}{2\ln 2}\Bigg[2\sum_{\alpha\beta} \langle\sigma_i^\alpha\rangle\langle\sigma_j^\beta\rangle\langle\sigma_i^\alpha\sigma_j^\beta\rangle \\
&\quad + \sum_{\alpha\neq\beta\neq\gamma} \bigg(\langle\sigma_i^\alpha\sigma_j^\alpha\rangle\langle\sigma_i^\beta\sigma_j^\gamma\rangle\langle\sigma_i^\gamma\sigma_j^\beta\rangle - \frac{2}{3}\langle\sigma_i^\alpha\sigma_j^\beta\rangle\langle\sigma_i^\beta\sigma_j^\gamma\rangle\langle\sigma_i^\gamma\sigma_j^\alpha\rangle \\
&\quad - \frac{1}{3}\langle\sigma_i^\alpha\sigma_j^\alpha\rangle\langle\sigma_i^\beta\sigma_j^\beta\rangle\langle\sigma_i^\gamma\sigma_j^\gamma\rangle \bigg) \Bigg] + o(\langle\cdots\rangle^4).
\end{aligned} \tag{14}
$$

Equation (14) indicates that the correlation entropy are the summation of the correlation functions with terms of powers larger than or equal to the second order.

To the spin-1/2 systems, the maximum of correlation functions with two nearest neighbor sites is 1/4. Furthermore, the values of correlation functions are decreasing with the increasing distances between two sites. Therefore, the correlation functions between two sites with the longest distance are small. These ensure that the values of nth power of correlation functions are larger than that of $(n+1)$th power, and the square terms are much larger than the nth power terms. To some systems such as the 2D quantum XY model which will be demonstrated in the following section, the contributions of second-order correlations to the correlation entropy (14) are much larger than that of the third and higher order correlations. In this case, the second-order correlations are the dominant terms and the higher order correlations are the correction to the results. (Please see table 1.)

Generally, near the critical temperature, the universal scaling law of the correlation function takes the following form:

$$C(r) \sim r^{-p}\,\mathrm{e}^{-r/\xi}, \tag{15}$$

where $r = |i - j|$ is the distance between two sites, p is the power exponent and ξ is the correlation length, which is a function of temperature T. The critical behavior of ξ is described by its critical exponent ν usually in the following form:

$$\xi \sim |t|^{-\nu}, \tag{16}$$

where $t = (T - T_\mathrm{c})/T_\mathrm{c}$ is the reduced temperature and T_c is the critical temperature. At the critical point T_c, the correlation length tends to infinity, which means that $\mathrm{e}^{-r/\xi} \to 1$ for any distance r. Thus the correlation function takes the form of

$$C(r) \sim 1/r^{p} \equiv 1/r^{d-2+\eta}, \tag{17}$$

where d is the dimension of the system and η is the critical exponent of the correlation function, which describes the decaying behavior of correlation effects with respect to the spatial distance r. At the critical point, the decay of correlation function is very slow. One character of the phase transition is that the correlation length is infinity at the critical point, while keeps a finite value at other points.

Close to the critical point, the entropy correlation length ζ is defined by

$$S(0:r) \sim r^{-q}\mathrm{e}^{-r/\zeta}, \tag{18}$$

where q is the power exponent. The ζ is the characteristic length of the entropy correlation effects, and it describes the length scale of correlation between two subsystems from the view of entropy. Close to the critical point, the entropy correlation length keeps a finite value then the decay of the correlation entropy satisfies the exponential law, where the leading term is $\mathrm{e}^{-r/\zeta}$. While at the critical point, the entropy correlation length tends to infinity and the decay of the correlation entropy satisfies the power law, where the leading term is $1/r^{d-2+\delta}$ and δ is the critical exponent of the correlation entropy. Therefore, the correlation entropy catches some intrinsic characters of the phase transitions and can be used to determine the phase transition points. Moreover, because the correlation entropy is a reasonable combination of correlation effects, the correlation entropy should have its own scaling behavior near the critical point.

3. The KT phase transition

We consider the 2D quantum XY model defined by the Hamiltonian

$$H = -J\sum_{\langle i,j\rangle}\left(S_i^x S_j^x + S_i^y S_j^y\right), \tag{19}$$

where J is the coupling constant, $S_i^x\left(S_i^y\right)$ is the spin-1/2 operator along the $x(y)$ direction at site i on a 2D $L \times L$ square lattice in space. We use the periodic boundary conditions. It is well

Table 1. The contributions of the second- and fourth-order correlations to the correlation entropy, where $T = 0.35$ (left) and $T = 0.40$ (right).

L	γ_x^2	$\frac{2}{3}\gamma_x^4$	Ratio	L	γ_x^2	$\frac{2}{3}\gamma_x^4$	Ratio
10	0.160 19	0.017 11	0.106 80	10	0.133 55	0.011 89	0.089 03
12	0.149 13	0.014 83	0.099 42	12	0.120 54	0.009 69	0.080 36
16	0.133 01	0.011 80	0.088 68	16	0.102 00	0.006 94	0.068 00
20	0.121 28	0.009 81	0.080 85	20	0.088 01	0.005 16	0.058 67
24	0.113 14	0.008 53	0.075 43	24	0.077 81	0.004 04	0.051 87
28	0.106 62	0.007 58	0.071 08	28	0.070 14	0.003 28	0.046 76
32	0.101 16	0.006 82	0.067 44	32	0.063 22	0.002 66	0.042 15

known that the model (19) has a KT transition at the critical point $T_{\mathrm{KT}} = 0.34J/k_B$ [31–33], where k_B is the Boltzmann constant. In the following, J and k_B are set to 1. At the critical point, the decay of correlation length of the KT transition satisfies the exponential law, instead of the usual power type (16). The thermodynamical quantities do not show any singularity at the critical temperature. Several quantities have been used to study this transition such as the superfluid density or equivalently the helicity modulus [33], correlation function and susceptibility [31, 32]. In this paper, we use the correlation entropy.

From the symmetry analysis, we obtain the two-site reduced density matrix as

$$\rho_{ij} = \frac{1}{4}I + \sum_{\alpha} \gamma_\alpha S_i^\alpha S_j^\alpha, \tag{20}$$

with $\alpha = x, y, z$ and $\gamma_\alpha = 4\langle S_i^\alpha S_j^\alpha \rangle$. The value of correlation function along the z-direction is not zero, although the Hamiltonian (19) does not include this kind of terms. The reduced density matrix ρ_{ij} can be diagonalized with the eigenvalues

$$\lambda_{1,2} = \tfrac{1}{4}(1 + \gamma_z \pm (\gamma_x - \gamma_y)), \qquad \lambda_{3,4} = \tfrac{1}{4}(1 - \gamma_z \pm (\gamma_x + \gamma_y)). \tag{21}$$

The single-site reduced density matrix is the unit matrix with the coefficient 1/2, and the partial entropy of a single site is 1. Then we obtain the correlation entropy as

$$S(i:j) = 2 + \sum_{n=1}^{4} \lambda_n \log_2 \lambda_n. \tag{22}$$

The correlation entropy (22) can also be written as

$$S(i:j) = \frac{1}{2\ln 2}\sum_{\alpha}\gamma_\alpha^2 + \frac{1}{\ln 2}\gamma_x\gamma_y\gamma_z + \frac{1}{12\ln 2}\left[\sum_{\alpha}\gamma_\alpha^4 + 3\sum_{\alpha\neq\beta}\gamma_\alpha^2\gamma_\beta^2\right] + o(\langle\cdots\rangle^5). \tag{23}$$

From equation (23), we see that the third-order correlations are the productions of correlation functions along the x, y and z directions. In the 2D XY model, the correlation functions along the x and y directions are equal, and they are much larger than that along the z-direction, $\langle S_i^x S_j^x\rangle = \langle S_i^y S_j^y\rangle \gg \langle S_i^z S_j^z\rangle$. Thus the third-order correlations are infinitesimal and equation (23) becomes

$$S(i:j) = \frac{1}{\ln 2}\left(\gamma_x^2 + \frac{2}{3}\gamma_x^4\right) + o(\langle\cdots\rangle^5). \tag{24}$$

We list the contributions of the second- and fourth-order correlations to the correlation entropy (24) in the table 1. From it, we see that the contributions of the second-order terms are much larger than that of the fourth-order terms. Furthermore, the ratio of fourth-order terms to second-order terms is decreasing with the increasing system size and the increasing distance between two sites. For example, the ratio is about 0.08 for the case of $L = 10$, and is about 0.04 for the case of $L = 32$, where the temperature $T = 0.4$. Therefore, it is reasonable to neglect the fourth and higher order terms.

For a $L \times L$ system with the periodic boundary condition and near the critical point, we assume that the correlation entropy $S(0 : r)$ and the corresponding entropy correlation length ζ have the following finite-size scaling behavior:

$$S_L(r) = A\left[r^{-\delta} D\left(\frac{r}{\zeta}\right) + (L-r)^{-\delta} D\left(\frac{L-r}{\zeta}\right)\right], \tag{25}$$

$$\zeta = A' \exp\left(\frac{B}{\sqrt{T - T_c}}\right), \qquad T \to T_c^+, \tag{26}$$

where $S(r) \equiv S(0 : r)$. Below the critical point, the system (19) has the quasi-long-range order and the ζ is always infinity. At the critical point, the entropy correlation length ζ is exponential divergence (26). In [31], the correlation function with different distances are calculated to extract the correlation length, which requires that the system size is very large. Here, in order to see the entropy correlation effects more clearly, we consider the correlation entropy of two sites with the longest distances $\vec{r} = (L/2, L/2)$ for the different system sizes $L \times L$. From equation (25), the correlation entropy $S[(0, 0) : (L/2, L/2)] \equiv S(L/2)$ has the scaling form of

$$S(L/2) \sim L^{-\delta} G(L/\zeta), \tag{27}$$

where $G(x)$ is the universal function. At the critical temperature, the entropy correlation length tends to infinity and $G(0)$ is a constant which does not depend on the system size L. We have

$$S(L/2) \sim L^{-\delta}, \qquad T = T_c. \tag{28}$$

Equations (26)–(28) are the main scaling laws of the correlation entropy for the KT transition.

Now, we calculate the correlation entropy by the QMC simulation, where the SSE method with operator-loop update [19–21] is used. The SSE method is based on the exact power-series expansion of $e^{-\beta H}$ without any systematic errors, where $\beta = 1/T$. To construct the configuration space of SSE, we rewrite the Hamiltonian (19) as

$$H = -\sum_{b=1}^{M} (H_{1b} + H_{2b} + H_{3b}), \tag{29}$$

where b is the bond connecting two spins with nearest neighbor and $M = 2L^2$. The partition function of the system can be expanded as

$$Z = \sum_{\alpha} \sum_{s_N} \frac{\beta^n (N-n)!}{N!} \langle\alpha| \prod_{i=1}^{N} H_{a_i, b_i} |\alpha\rangle, \tag{30}$$

where $\{|\alpha\rangle\}$ is a complete set of the basis, N is the truncation, s_N is a sequence of operator indices

$$s_N = [a_1, b_1][a_2, b_2] \cdots [a_N, b_N], \tag{31}$$

with $a_i \in \{1, 2, 3\}$, $b_i \in \{1, \ldots, M\}$ or $[a_i, b_i] = [0, 0]$ and n is the total number of operators with non-[0, 0] indices. The sampling schemes are developed according to the operator's

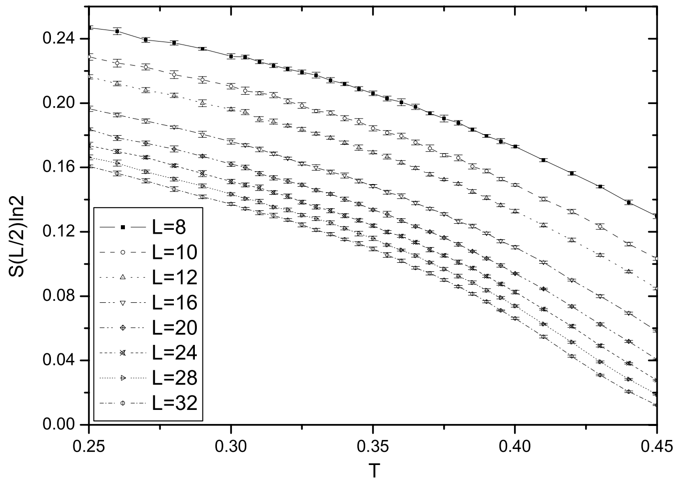

Figure 1. The correlation entropy for different system sizes versus the temperature. We see that the correlation entropy does not have any singularity in the temperature region $0.25 < T < 0.45$.

relative weight in the partition function (30). The correlation between two diagonal operators $\hat{D}_1$ and $\hat{D}_2$ is quantified by

$$\langle \hat{D}_1 \hat{D}_2 \rangle = \left\langle \frac{1}{n+1} \sum_{k=0}^{n} d_1[k] d_2[k] \right\rangle, \tag{32}$$

where $d_i[k] = \langle \alpha(k)|\hat{D}_i|\alpha(k)\rangle$ and $|\alpha(k)\rangle \sim \prod_{i=1}^{k} H_{a_i,b_i}|\alpha\rangle$. When calculating the transverse correlation functions $\langle S_i^x S_j^x \rangle$, it is convenient to choose the basis $|\alpha\rangle$ as the eigenstate of S^x and the decomposition of Hamiltonian (19) is

$$\begin{aligned} H_{1b} &= C + S^x_{i(b)} S^x_{j(b)}, \\ H_{2b} &= \tfrac{1}{4}\left(S^+_{i(b)} S^+_{j(b)} + S^-_{i(b)} S^-_{j(b)}\right), \\ H_{3b} &= \tfrac{1}{4}\left(S^+_{i(b)} S^-_{j(b)} + S^-_{i(b)} S^+_{j(b)}\right), \end{aligned} \tag{33}$$

where $S_j^{\pm} = S_j^y \pm \mathrm{i} S_j^z$ are the spin-flipped operators along the x-direction at the site j. The constant C is chosen to ensure a positive weight of H_{1b} in the expansion of the partition function. While when calculating the correlation function $\langle S_i^z S_j^z \rangle$, $|\alpha\rangle$ is chosen as the eigenstate of S^z and the decomposition the Hamiltonian (19) is simple. $H = -\sum_{b=1}^{M}(H_{1b} + H_{2b})$, where $H_{1b} = C$, $H_{2b} = \left(\tilde{S}^+_{i(b)} \tilde{S}^-_{j(b)} + \tilde{S}^-_{i(b)} \tilde{S}^+_{j(b)}\right)/4$ and $\tilde{S}_j^{\pm} = S_j^x \pm \mathrm{i} S_j^y$ are the spin-flipped operators in the z-direction at the site j.

The results are the following. The correlation entropy $S(L/2)$ for the system sizes $L = 8 - 32$ versus the temperature is shown in figure 1. From it, we see that the correlation entropy does not have any singularity in the temperature region $0.25 < T < 0.45$. The finite-size scaling behavior of the correlation entropy is shown in figure 2. We find that the data from $L = 10$ to $L = 32$ fall on a single curve while the data for $L = 8$ depart from that curve. Thus, the system enters the scaling region only in the case of $L \geqslant 10$. From figure 2,

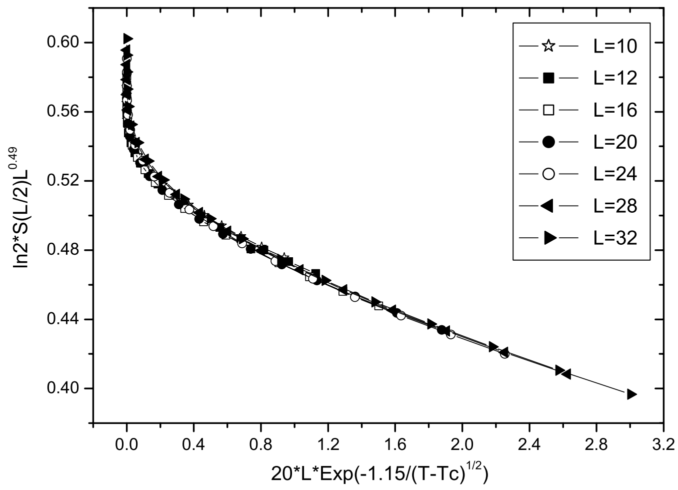

Figure 2. The finite-size scaling behavior of the correlation entropy. All the data from $L = 10$ to $L = 32$ fall on a single curve. The data for $L = 8$ does not satisfy the scaling law. Therefore, the system enters the scaling region only in the case of $L \geqslant 10$.

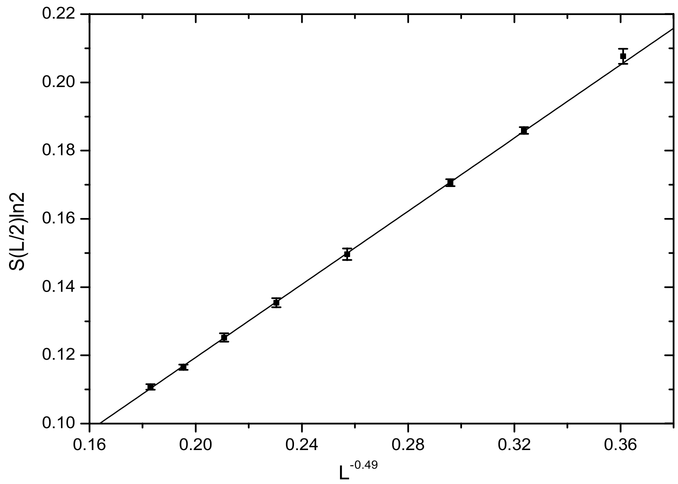

Figure 3. The finite-size scaling behavior of correlation entropy at the critical temperature T_c. The data for $L = 10 - 32$ are fit as a straight line with the slope 0.53(6), which agrees with equation (28). The data for $L = 8$ is slightly above the line, which means that the system does not enter the scaling region at that size.

we also obtain the critical temperature and the critical exponents as

$$
\begin{aligned}
&T_c = 0.348 \pm 0.002, \\
&\delta = 0.490 \pm 0.003, \\
&\zeta \sim \exp(1.15/\sqrt{T - T_c}).
\end{aligned}
\tag{34}
$$

At the critical temperature, the curve of correlation entropy $S(L/2)$ versus the system-size scaling $L^{-\delta}$ is a straight line, which is shown in figure 3. The data for $L = 8$ is slightly above the line, which means that the correlation entropy does not enter the scaling region at that system size. At the critical point, the correlation function satisfies $C(L/2) \sim L^{-\eta}$ with the critical exponent $\eta = 0.249(76)$ [31], while the correlation entropy gives $S(L/2) \sim L^{-\delta}$ with the critical exponent $\delta = 0.49$. Comparing δ and η, we find that the critical exponent of correlation entropy is approximately twice as large as the critical exponent of correlation function, $\delta \approx 2\eta$, which consists with the analytic results (24).

All these results agree with the previous studies on the KT transition [31–33]. For example, in [31] the correlation functions with different distances r are calculated and gives the critical temperature as $T_c = 0.353(3)$. In [32], from the calculation of the susceptibility, the critical temperature is obtained as $T_c = 0.3433$. In [33], by using the high accurate QMC simulation and the helicity modulus, the critical temperature is determined as $T_c = 0.3422$.

4. Summary

In summary, we show that the correlation entropy can be used as a measure to quantify the quantum and finite-temperature phase transitions. We obtain a relation between the correlation entropy and the correlation function for the general spin-1/2 systems. We find that the entropy correlation length is approximately half of the correlation length if the third and higher order correlations can be neglected. This method has many advantages and is valid for the topological phase transitions. As an example, the KT transition in the quantum 2D XY model is studied. The critical temperature and the critical exponents are determined from the finite-size scaling analysis of the correlation entropy. We hope some hidden phase transitions and quantum coherence can be found by this method.

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References

[1] Osterloh A, Amico L, Falci G and Fazio R 2002 *Nature* **416** 608
[2] Osborne T J and Nielsen M A 2002 *Phys. Rev.* A **66** 032110
[3] Gu S J, Deng S S, Li Y Q and Lin H Q 2004 *Phys. Rev. Lett.* **93** 086402
[4] Cao J, Cui X, Qi Z, Lu W, Niu Q and Wang Y 2007 *Phys. Rev.* B **75** 172401
[5] Vidal G, Latorre J I, Rico E and Kitaev A 2003 *Phys. Rev. Lett.* **90** 227902
[6] Barnum H, Knill E, Ortiz G and Viola L 2003 *Phys. Rev.* A **68** 032308
[7] Verstraete F, Popp M and Cirac J I 2004 *Phys. Rev. Lett.* **92** 027901
[8] Somma R, Ortiz G, Barnum H, Knill E and Viola L 2004 *Phys. Rev.* A **70** 042311
[9] Roscilde T, Verrucchi P, Fubini A, Haas S and Tognetti V 2004 *Phys. Rev. Lett.* **93** 167203
[10] Popp M, Verstraete F, Martín-Delgado M A and Cirac J I 2005 *Phys. Rev.* A **71** 042306
[11] Roscilde T, Verrucchi P, Fubini A, Haas S and Tognetti V 2005 *Phys. Rev. Lett.* **94** 147208
[12] Gu S J, Lin H Q and Li Y Q 2003 *Phys. Rev.* A **68** 042330
[13] Kosterlitz J M and Thouless D J 1973 *J. Phys. C: Solid State Phys.* **6** 1181
[14] Kosterlitz J M 1974 *J. Phys. C: Solid State Phys.* **7** 1046
[15] Doniach S 1981 *Phys. Rev.* B **24** 5063
[16] Jacobs L, José J V, Novotny M A and Goldman A M 1988 *Phys. Rev.* B **38** 4562
[17] Williams G A 1987 *Phys. Rev. Lett.* **59** 1926
Williams G A 1988 *Phys. Rev. Lett.* **61** 1142
[18] Chattopadhyay B and Shenoy S R 1994 *Phys. Rev. Lett.* **72** 400
[19] Sandvik A W 1999 *Phys. Rev.* B **59** R14157
[20] Sandvik A W and Kurkijärvi J 1991 *Phys. Rev.* B **43** 5950

[21] Sandvik A W 1997 *Phys. Rev.* B **56** 11678
[22] Vedral V 2002 *Rev. Mod. Phys.* **74** 197
[23] Anfossi A, Giorda P, Montorsi A and Traversa F 2005 *Phys. Rev. Lett.* **95** 056402
[24] Anfossi A, Giorda P and Montorsi A 2007 *Phys. Rev.* B **75** 165106
[25] Gu S J, Sun C P and Lin H Q 2006 *Preprint* quant-ph/0605164
[26] Groisman B, Popescu S and Winter A 2005 *Phys. Rev.* A **72** 032317
[27] Adami C and Cerf N J 1997 *Phys. Rev.* A **56** 3470
[28] Stratonovich R L 1966 *Probl. Inf. Transm.* **2** 35
[29] Vedral V, Plenio M B, Rippin M A and Knight P L 1997 *Phys. Rev. Lett.* **78** 2275
[30] Vedral V, Rippin M A and Plenio M B 1997 *J. Mod. Opt.* **44** 2185
[31] Ding H Q 1992 *Phys. Rev.* B **45** 230
[32] Ding H Q and Makivic M S 1990 *Phys. Rev.* B **42** 6827
[33] Harada K and Kawashima N 1997 *Phys. Rev.* B **55** R11949