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2008 J. Phys. A: Math. Theor. 41 025002

(http://iopscience.iop.org/1751-8121/41/2/025002)

IOP PUBLISHING JOURNAL OF PHYSICS A: MATHEMATICAL AND THEORETICAL

J. Phys. A: Math. Theor. **41** (2008) 025002 (18pp) doi:10.1088/1751-8113/41/2/025002

Universal role of correlation entropy in critical phenomena

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Received 5 September 2007, in final form 18 November 2007
Published 19 December 2007
Online at stacks.iop.org/JPhysA/41/025002

Abstract
In statistical physics, if we divide successively an equilibrium system into two parts, we will face a situation that, to a certain length ξ, the physics of a subsystem is no longer the same as the original one. The extensive property of the thermal entropy $S(\mathrm{A} \cup \mathrm{B}) = S(\mathrm{A}) + S(\mathrm{B})$ is then violated. This observation motivates us to introduce a concept of correlation entropy between two points, as measured by the mutual information in information theory, to study the critical phenomena. A rigorous relation is established to display some drastic features of the non-vanishing correlation entropy of a subsystem formed by any two distant particles with long-range correlation. This relation actually indicates a universal role played by the correlation entropy for understanding the critical phenomena. We also verify these analytical studies in terms of two well-studied models for both the thermal and quantum phase transitions: the two-dimensional Ising model and the one-dimensional transverse-field Ising model. Therefore, the correlation entropy provides us with a new physical intuition of the critical phenomena from the point of view of information theory.

PACS numbers: 05.70.Jk, 75., 75.10.Hk

(Some figures in this article are in colour only in the electronic version)

1. Introduction

Entropy is one of the most important concepts in both statistical physics [1] and information theory [2–4]. It measures how much uncertainty is there in a state of a physical system. In statistical physics, the entropy defined by $S = \log_2 \Omega$ depends on the number of states Ω in an equilibrium system; while in information theory, the entropy $S = -\mathrm{tr}(\rho \log_2 \rho)$ is associated with the probability distribution in the eigenstate space of a density matrix ρ. Therefore, it is very interesting to look into some fundamental issues from different points of view due to the common ground of two fields.

In statistical physics, if we divide an equilibrium system into a large number of macroscopic parts, the total number of state in the phase space is a product of the number of state ω_i of each part, i.e. $\Omega = \prod_i \omega_i$. This precondition leads to the fact that the entropy is an extensive quantity in statistical physics, i.e. $S = \sum_i S_i$, which is one of the bases of the second law of the thermodynamics. However, a realistic system includes all kinds of interactions, and the dynamics at one site is no longer independent of other sites nearby. This fact implies that if we successively divide a system into two parts, we will face a situation that, to a certain length ξ, the physics of a subsystem is no longer the same as the original one. The length ξ actually defines a characteristic scale for the statistical physics, and physicists usually call it correlation length in studies of different kinds of correlation functions. From the point of view of information theory, for two subsystems A and B within the length scale ξ, they are no longer independent of each other, and their entropy does not satisfy the extensive property[3], i.e., $S(\mathrm{A} \cup \mathrm{B}) \neq S(\mathrm{A}) + S(\mathrm{B})$.

On the other hand, the correlation function plays a fundamental role in physics. Almost all physical quantities, not only in condensed matter physics but also in quantum field theory, are related to the correlation function. Thus, it devotes to understanding many phenomena in quantum mechanics. Physically, the correlation function denotes the amplitude of the dependence of physical variables between two points in spacetime. From the point of view of information theory, it also partially measures how much uncertainty of a physical quantity is at one location if the quantity at another location is given. However, this uncertainty still depends on the quantity itself. For example, in the quantum system, the diagonal correlation function usually differs from the off-diagonal correlation function. Therefore, in order to learn the dependence between two separated systems, it is important to ask such a question: to what extent the equality $S(\mathrm{A} \cup \mathrm{B}) = S(\mathrm{A}) + S(\mathrm{B})$ is violated. This question introduces an important concept in information theory, i.e., the mutual information, which is defined as

$$S(\mathrm{A}|\mathrm{B}) = S(\mathrm{A}) + S(\mathrm{B}) - S(\mathrm{A} \cup \mathrm{B}), \tag{1}$$

where $S(i) = -\mathrm{tr}(\rho_i \log_2 \rho_i)$, $i = \mathrm{A}, \mathrm{B}, \mathrm{A} \cup \mathrm{B}$ is the entropy of the corresponding reduced density matrix. If ρ is classical, it is the Shannon entropy [2]; otherwise it is the von Neumann entropy [5] of quantum information theory. Actually, all correlation functions $\langle O_\mathrm{A} O_\mathrm{B} \rangle$ between subsystems A and B can be calculated from the reduced density matrix $\rho_{\mathrm{A}\cup\mathrm{B}}$, i.e., $\langle O_\mathrm{A} O_\mathrm{B} \rangle = \mathrm{tr}\langle O_\mathrm{A} O_\mathrm{B} \rho_{\mathrm{A}\cup\mathrm{B}} \rangle$. The mutual information, which measures the common shared information, defines a more general operator-independent correlation between two subsystems. Taking into account the role of entropy in the statistical physics, we would like to call it correlation entropy hereafter.

To have a concrete interpretation, let us resort to the original understanding of the entropy. In information theory, the entropy is used to quantify the physical resource (in units of classical bit due to $\log_2$ in its expression) needed to store information. For example, in the exact diagonalization approach, if we want to diagonalize a Hamiltonian of 10-site spin-1 chain and no symmetry can be used to reduce the dimension of its Hilbert space, we need at least $S = \log_2 3^{10} = 10 \log_2 3$ bits to store a basis. Therefore, the correlation entropy actually measures the additional physical resource required if we store two subsystems, respectively, rather than store them together. As a simple example, let us consider a two-qubit system in a singlet state $(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)/\sqrt{2}$, we have $S(\mathrm{A}) = 1$, $S(\mathrm{B}) = 1$, $S(\mathrm{A} \cup \mathrm{B}) = 0$, which leads to $S(\mathrm{A}|\mathrm{B}) = 2$. Obviously, there is no information in a given singlet state. However, each spin in this state is completely uncertain. So we need two bits to store them respectively. On the

[3] In information theory 'extensivity' property of the mutual entropy is usually called 'additivity'

other hand, the correlation entropy is simply twice the entanglement, as measured by partial entropy, between two systems because of $S(\mathrm{A}) = S(\mathrm{B})$ for a pure state. The reason why we interpret the correlation entropy in this way is that besides the quantum correlation the state also has classical correlation [6]. From this point of view, the correlation entropy is just a measure of total correlation, including the quantum and classical correlations, between two subsystems. They go halves with each other in correlation entropy for the pure state. For a mixed state, the correlation entropy also measures the amount of the uncertainty of one system before we learn one from another. From the above interpretations, it is then not surprising that the correlation entropy fails to measure the entanglement [7].

In the statistical physics, the critical phenomena are the central topic. To have a complete understanding on the critical behavior, various methods, such as renormalization group [8], Monte–Carlo simulation [9] and mean-field approach, etc, have been developed and applied to many kinds of systems. In recent years, the study on the role of entanglement [10–15] as well as the quantum mutual information [16] in the quantum critical behavior [17] has established a bridge between quantum information theory and condensed matter physics, and sheds new light on the quantum phase transitions due to its interesting behavior around the critical point. However, the entanglement is fragile under the thermal fluctuation and can be suppressed to zero at finite temperatures. Then it is difficult to witness a generalized thermal phase transition in terms of quantum entanglement.

In this paper, we will study the role of the correlation entropy in both thermal and quantum phase transitions. Like the fundamental role of the two-point correlation function in the statistical physics, we are interested in the universal role played by the two-point correlation entropy in critical phenomena. The paper is organized as follows. In section 2, for a pedagogical purpose, we study a toy model, i.e., the Heisenberg dimer, and show that the thermal entropy is not an extensive parameter in such a simple system. In section 3, we discuss the relation between the reduced density matrix, the long-range correlation and the correlation entropy. In section 4, we study the properties of the correlation entropy in thermal phase transition, as illustrated by the classical two-dimensional Ising model. In section 5, we study the properties of the correlation entropy in a simple quantum phase transition of the one-dimensional transverse-field Ising model. In section 6, some discussions and prospects are presented. Finally, a brief summary is given in section 7.

2. A toy model: Heisenberg dimer

For a pedagogical purpose and making our motivation more clear, we first have a look at a toy model: Heisenberg dimer, whose Hamiltonian reads

$$H = \sigma_1 \cdot \sigma_2, \tag{2}$$

where $\sigma_i(\sigma^x, \sigma^y, \sigma^z)$ are Pauli matrices at site i,

$$\sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{3}$$

and the coupling between the two sites is set to unit for simplicity. The Hamiltonian can be diagonalized easily. Its ground state is a spin singlet state

$$\Psi_0 = \frac{1}{\sqrt{2}}\left[|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right], \tag{4}$$

with eigenvalue $E_0 = -3$, while three degenerate excited states are

$$\Psi_1 = \frac{1}{\sqrt{2}}[|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle], \qquad \Psi_2 = |\uparrow\uparrow\rangle, \Psi_3 = |\downarrow\downarrow\rangle, \tag{5}$$

with higher eigenvalue $E_{1,2,3} = 1$. Therefore, according to the statistical physics, the thermal entropy of the system vanishes at zero temperature. When the system is contacted with a thermal bath with temperature T, the thermal state of the system is described by a density matrix

$$\rho = \zeta \begin{pmatrix} \mathrm{e}^{-2/T} & 0 & 0 & 0 \\ 0 & \cosh(2/T) & -\sinh(2/T) & 0 \\ 0 & -\sinh(2/T) & \cosh(2/T) & 0 \\ 0 & 0 & 0 & \mathrm{e}^{-2/T} \end{pmatrix} \tag{6}$$

where

$$\zeta = \frac{1}{3\mathrm{e}^{-2/T} + \mathrm{e}^{2/T}}. \tag{7}$$

Because of SU(2) symmetry of the Heisenberg dimer, the single-site entropy $S(i)$ of the system is always unity, and the entropy of the whole system is

$$S(1 \cup 2) = \frac{\log_2(3\mathrm{e}^{-4/T} + 1)}{3\mathrm{e}^{-4/T} + 1} + \frac{3\log_2(3 + \mathrm{e}^{4/T})}{3 + \mathrm{e}^{4/T}}. \tag{8}$$

Then we can see that $S(1 \cup 2) \neq S(1) + S(2)$ both at zero and finite temperatures. In the high-temperature limit, the asymptotic behavior of the correlation entropy is $S(1|2) \propto 1/T^2$. So only when $T \to \infty$, $S(1|2) \to 0$, the extensive property then holds. The physics behind this fact is quite clear. It is the interaction between the two sites that establishes a kind of correlation and then breaks the extensive property of the entropy.

For a large system, however, the correlation entropy usually decays with the increasing of distance between the two parts, and the entropy becomes an extensive quantity beyond the characteristic scale. Only around the critical point where a phase transition occurs, does the system behave like a whole and cannot be divided into two parts, and then the correlation entropy has long-range behavior.

3. Reduced density matrix, long-range order and correlation entropy

In many-body physics, the reduced density matrices of a one- and two-body subsystem can be, in general, written as

$$\langle \mu' | \rho_i | \mu \rangle = \mathrm{tr}\big(a_{i\mu'} \rho a_{i\mu}^\dagger\big), \qquad \langle \mu' \nu' | \rho_{i\cup j} | \mu\nu \rangle = \mathrm{tr}\big(a_{i\mu'} a_{j\nu'} \rho a_{j\nu}^\dagger a_{i\mu}^\dagger\big), \tag{9}$$

respectively. Here, $a_{i\mu}, a_{j\nu}$ are annihilation operators for states $|\mu\rangle, |\nu\rangle$ localized at site i, j, respectively, and satisfy the commutation (anti-commutation) relation for bosonic (fermionic) states. The reduced density matrices are usually normalized as

$$\mathrm{tr}(\rho_i) = 1, \qquad \mathrm{tr}(\rho_{i\cup j}) = 1, \tag{10}$$

so that one has a probability explanation for their diagonal elements in the corresponding eigenstate space.

In the spin system, the reduced density matrix of a single spin at position i takes the form

$$\rho_i = \tfrac{1}{2}\big(1 + \langle \sigma_i^x \rangle \sigma_i^x + \langle \sigma_i^y \rangle \sigma_i^y + \langle \sigma_i^z \rangle \sigma_i^z\big). \tag{11}$$

For two arbitrary spins at positions i and j, the two-site reduced density matrix generally takes the form

$$\rho_{i\cup j} = \frac{1}{4} + \frac{1}{4}\sum_\mu \big(\langle \sigma_i^\mu \rangle \sigma_i^\mu + \langle \sigma_j^\mu \rangle \sigma_j^\mu\big) + \frac{1}{4}\sum_{\mu\nu} \langle \sigma_i^\mu \sigma_j^\nu \rangle \sigma_i^\mu \sigma_j^\nu. \tag{12}$$

Obviously, under some symmetry, the above reduced density matrix can be simplified. For example, if the state of N spins is also an eigenstate of z-component of total spins $S^z = \sum S_i^z = 0$ and possesses the exchange symmetry, then equation (12) can be simplified as

$$\rho_{i\cup j} = \begin{pmatrix} u^+ & 0 & 0 & 0 \\ 0 & w_1 & z & 0 \\ 0 & z^* & w_2 & 0 \\ 0 & 0 & 0 & u^- \end{pmatrix} \tag{13}$$

in the basis of $\sigma_i^z\sigma_j^z$: $\{|\uparrow\uparrow\rangle, |\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle, |\downarrow\downarrow\rangle\}$. Here, the matrix elements can be calculated from the correlation functions

$$\begin{aligned} u^+ &= u^- = \tfrac{1}{4}\left(1 + \left\langle\sigma_i^z\sigma_j^z\right\rangle\right), \\ w_1 &= w_2 = \tfrac{1}{4}\left(1 - \left\langle\sigma_i^z\sigma_j^z\right\rangle\right), \\ z &= \tfrac{1}{4}\left(\left\langle\sigma_i^x\sigma_j^x\right\rangle + \left\langle\sigma_i^y\sigma_j^y\right\rangle\right). \end{aligned} \tag{14}$$

With the help of the Jordan–Schwinger mapping [18],

$$\sigma_j^+ = a_{j\uparrow}^\dagger a_{j\downarrow}, \qquad \sigma_j^- = a_{j\downarrow}^\dagger a_{j\uparrow}, \qquad \sigma_j^z = \left(a_{j\uparrow}^\dagger a_{j\uparrow} - a_{j\downarrow}^\dagger a_{j\downarrow}\right) \tag{15}$$

where $a_{j\mu}^\dagger$ stands for the pseudo fermionic creation operator for single-particle state $|j,\mu\rangle$ at position j; the element in the reduced density matrix (12) can be reexpressed in the form of equation (9). For example,

$$\left\langle\sigma_i^+\sigma_j^-\right\rangle = -\left\langle a_{i\uparrow}^\dagger a_{j\downarrow}^\dagger a_{i\downarrow} a_{j\uparrow}\right\rangle. \tag{16}$$

Therefore, we can explore the property of long-range correlation in the spin system through pseudo fermion systems.

We first consider the long-range correlation in classical systems, e.g. Ising model, in which the reduced density matrices take the diagonal form, i.e.

$$\begin{aligned} \langle\mu'|\rho_i|\mu\rangle &= \delta_{\mu'\mu}\,\mathrm{tr}\left(a_{i\mu'}\rho a_{i\mu}^\dagger\right), \\ \langle\mu'\nu'|\rho_{i\cup j}|\mu\nu\rangle &= \delta_{\mu'\mu}\delta_{\nu'\nu}\,\mathrm{tr}\left(a_{i\mu'}a_{j\nu'}\rho a_{j\nu}^\dagger a_{i\mu}^\dagger\right). \end{aligned} \tag{17}$$

Then, if there is no long-range correlation

$$\begin{aligned} \langle\mu\nu|\rho_{i\cup j}|\mu\nu\rangle &= \mathrm{tr}\left(a_{j\nu}^\dagger a_{i\mu}^\dagger a_{i\mu} a_{j\nu}\rho\right), \\ &= \left\langle a_{j\nu}^\dagger a_{i\mu}^\dagger a_{i\mu} a_{j\nu}\right\rangle, \\ &\to \left\langle a_{i\mu}^\dagger a_{i\mu}\right\rangle\left\langle a_{j\nu}^\dagger a_{j\nu}\right\rangle, \end{aligned} \tag{18}$$

for $|i-j| \to \infty$, the two-site entropy becomes

$$S(i\cup j) \to S(i) + S(j), \tag{19}$$

where

$$S(l) = -\sum_\nu \left\langle a_{l\nu}^\dagger a_{l\nu}\right\rangle \log_2\left\langle a_{l\nu}^\dagger a_{l\nu}\right\rangle, \qquad l = i, j, \tag{20}$$

where the normalization conditions of $\rho_{i(j)}$ and $\rho_{i\cup j}$ have been used. Obviously, we have $S(i|j) = 0$, which means that if there is no long-range correlation, the correlation entropy vanishes at a long distance.

On the other hand, if there exists long-range correlation, for example,

$$G_{i\mu,j\nu} \equiv \langle n_{i\mu}n_{j\nu}\rangle - \langle n_{i\mu}\rangle\langle n_{j\nu}\rangle = C, \tag{21}$$

for $|i-j|\to\infty$ and a nonzero C, then

$$S(i|j) > 0. \tag{22}$$

Now we study the correlation entropy in quantum systems, in which the reduced density matrix usually is not diagonal. Then, if the system does not have long-range correlation,

$$\langle\mu'\nu'|\rho_{i\cup j}|\mu\nu\rangle = \langle a^\dagger_{i\mu}a_{i\mu'}\rangle\langle a^\dagger_{j\nu}a_{j\nu'}\rangle, \tag{23}$$

for $|i-j|\to\infty$, the reduced density matrix can be written into a direct product form, i.e.

$$\rho_{i\cup j} = \rho_i \otimes \rho_j. \tag{24}$$

Then the reduced density matrices ρ_i, ρ_j can be diagonalized in their own subspace. So in principle, we can have $\rho_i = \sum_\mu p_\mu|\varphi_\mu\rangle_{ii}\langle\varphi_\mu|$, and $\rho_j = \sum_\nu p_\nu|\varphi_\nu\rangle_{jj}\langle\varphi_\nu|$, where p_μ, p_ν are the probability distributions for ρ_i and ρ_j, respectively. As we have done for the classical system, we then have

$$S(i|j) = S(\rho_i) + S(\rho_j) - S(\rho_{i\cup j}) = 0. \tag{25}$$

In order to study its relation to the long-range correlation, now we express the correlation entropy in terms of the relative entropy [19]

$$S(i|j) = \mathrm{tr}(\rho_{i\cup j}\log_2\rho_{i\cup j}) - \mathrm{tr}(\rho_{i\cup j}\log_2\rho_i\otimes\rho_j) \tag{26}$$

between the whole system and the direct product form of two subsystems where $(\rho_i \otimes \rho_j)_{\mu\nu,\mu'\nu'} = \langle a^\dagger_{i\mu}a_{i\mu'}\rangle\langle a^\dagger_{j\nu}a_{j\nu'}\rangle$. Then if there exists a long-range correlation, such as

$$\langle\mu'\nu'|\rho_{ij}|\mu\nu\rangle = \langle a^\dagger_{i\mu}a_{i\mu'}\rangle\langle a^\dagger_{j\nu}a_{j\nu'}\rangle + C, \tag{27}$$

for $|i-j|\to\infty$ and a nonzero C, it can be proved that [20]

$$S(i|j) > 0. \tag{28}$$

In quantum information theory, inequality (28) is called Klein inequality [20]. Therefore, the existence of the long-range correlation will lead to a positive correlation entropy (28). This observation is very important in understanding critical phenomena. According to the theory of phase transitions, the presence of the long-range correlation is crucial. However, different phase transitions depend on the different long-range correlations. For example, in the superfluid phase of ^{4}He, the off-diagonal-long-range order, as suggested by Yang [21], is necessary; while in another kind of condensate of exciton, it may require a diagonal-long-range correlation [22]. Then the above results show that the non-vanishing positive-defined correlation entropy is a universal and necessary condition for general critical phenomena[4].

4. Thermal phase transition: the two-dimensional Ising model

The physics in the above toy model is quite limited. In order to verify our analytical results and see the significance of the correlation entropy in the critical phenomena, let us first study its properties in a thermodynamical system. One of the typical examples is the two-dimensional Ising model, which is certainly the most thoroughly researched model in statistical physics [23, 24].

In the absence of the external field, the model Hamiltonian defined on a square lattice reads

$$H = -\sum_{\langle \mathbf{ij}\rangle}\sigma^z_{\mathbf{i}}\sigma^z_{\mathbf{j}}, \tag{29}$$

[4] Those quantum phase transitions induced by the ground-state level-crossing in a small system are not included.

where the sum is over all pairs of nearest-neighbor sites $\mathbf{i}$ and $\mathbf{j}$, and the coupling is set to unit for simplicity. Since the Ising model is a classical model, the reduced density matrix of two arbitrary spins then takes the form

$$\rho_{\mathbf{i}\cup\mathbf{j}} = \begin{pmatrix} u^+ & 0 & 0 & 0 \\ 0 & w_1 & 0 & 0 \\ 0 & 0 & w_2 & 0 \\ 0 & 0 & 0 & u^- \end{pmatrix} \tag{30}$$

in which the elements can be calculated from equation (14), and the single-site reduced density matrix

$$\rho_{\mathbf{i}} = \frac{1}{2}\begin{pmatrix} 1 + \langle\sigma_i^z\rangle & 0 \\ 0 & 1 - \langle\sigma_i^z\rangle \end{pmatrix}. \tag{31}$$

For simplicity, we only consider the correlation entropy along (1, 1) direction, because the long distance behavior of the correlation entropy should be independent of directions.

According to the exact solution of the two-dimensional Ising model [24], the magnetization per site of the system is

$$\langle\sigma_{\mathbf{i}}^z\rangle = \begin{cases} [1 - \sinh^{-4}(2/T)]^{1/8} & T < T_c \\ 0 & T > T_c \end{cases} \tag{32}$$

where the critical temperature T_c is determined by

$$2\tanh(2/T) = 1, \tag{33}$$

then $T_c \simeq 2.269185$. The correlation function can be calculated as

$$\langle\sigma_{0,0}^z\sigma_{r,r}^z\rangle = \begin{vmatrix} a_0 & a_{-1} & \cdots & a_{-r+1} \\ a_1 & a_0 & \cdots & a_{-r+2} \\ \vdots & \vdots & \vdots & \vdots \\ a_{r-1} & a_{r-2} & \cdots & a_0 \end{vmatrix} \tag{34}$$

where

$$a_n = \frac{1}{2\pi}\int_0^{2\pi} \mathrm{d}\theta\, \mathrm{e}^{\mathrm{i}n\theta}\phi(\theta), \tag{35}$$

and

$$\phi(\theta) = \left[\frac{\sinh^2(2/T) - \mathrm{e}^{-\mathrm{i}\theta}}{\sinh^2(2/T) - \mathrm{e}^{\mathrm{i}\theta}}\right]^{1/2}. \tag{36}$$

Therefore, we can calculate the correlation entropy directly from the known results.

We show the correlation entropy $S(\mathbf{i}|\mathbf{j})$ as a function of temperature T and distance between two sites $\mathbf{r} = \mathbf{i} - \mathbf{j}$ in figure 1. The result is impressive. It is well known that the two-dimensional Ising model has two different phases separated by T_c. Below T_c, the system has macroscopic magnetization, i.e., spontaneously magnetized, and its mean magnetization is determined by equation (32). While above T_c, the thermal fluctuation destroys the order and the system becomes paramagnetic. Therefore, it is not difficult to understand that the correlation entropy between the two sites decays quickly as the distance increases. This fact implies that the extensive property of the entropy holds beyond a finite correlation length. So the physics in a small system can be used to describe that for a large system. It is also the reason why in the Monte–Carlo approach, a simulation on a small system at low temperature and higher temperature agrees with the analytic result in the thermodynamic limit excellently. However, in the critical region, as we can see from figure 1, the correlation entropy decays in

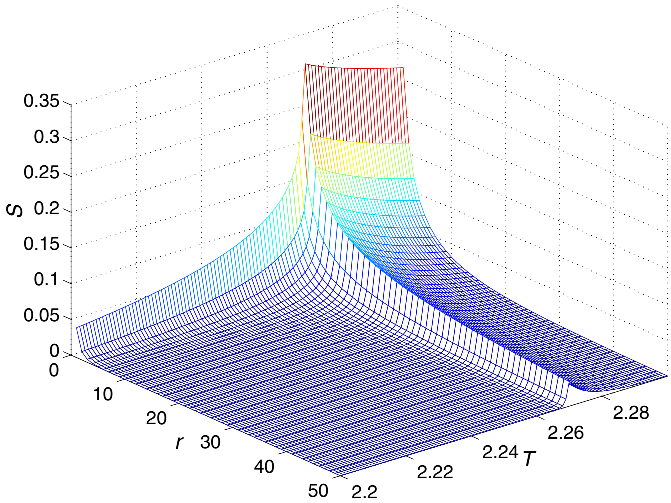

Figure 1. The correlation entropy as a function of temperature T (in units of Ising coupling) and the distance r (in units of $\sqrt{2}$ lattice constant).

a power-law way. This fact not only tells us a strong dependence between arbitrary two sites in the system, but also manifests the integrality of the whole system.

In the critical phenomena, scaling and universality are the most important themes [25, 26]. For the thermal phase transitions, the critical exponents [27] for specific heat C_v, order parameter σ^z, and susceptibility χ scale like

$$C_v \propto |T - T_c|^{-\alpha}, \qquad \langle \sigma^z \rangle \propto |T - T_c|^{\beta}, \qquad \chi \propto |T - T_c|^{-\gamma} \tag{37}$$

around the critical point T_c. The scaling analysis shows that the three critical exponents are not independent, but satisfy an interesting scaling relation [26]

$$\alpha + 2\beta + \gamma = 2. \tag{38}$$

For example, the critical exponents of the two-dimensional Ising model are $\alpha = 0$, $\beta = 1/8$ and $\gamma = 7/4$.

Clearly, the specific heat, the order parameter and the susceptibility actually depend only on two quantities, i.e., the internal energy and the order parameter itself. The internal energy is simply the thermal expectation value of the correlation function of the two neighboring spins, which is the main element of the two-site reduced density matrix (30). While the order parameter completely determines the single-site reduced density matrix (31). Below T_c, the correlation entropy is dominated by the order parameter, while above T_c, the correlation entropy is related to the internal energy. Therefore, if we consider the first-order derivative of the correlation entropy with respect to T below and above T_c, i.e.

$$\left.\frac{\partial S(\mathbf{i}|\mathbf{j})}{\partial T}\right|_{T<T_c}, \qquad \left.\frac{\partial S(\mathbf{i}|\mathbf{j})}{\partial T}\right|_{T>T_c} \tag{39}$$

we might have two different exponents α', β'. Furthermore, if we integrate the correlation entropy over the whole space, i.e.

$$\Theta = \int S(0,0|x,y)\,\mathrm{d}x\,\mathrm{d}y, \tag{40}$$

which is naturally related to the susceptibility; we use γ' to denote Θ's critical exponent.

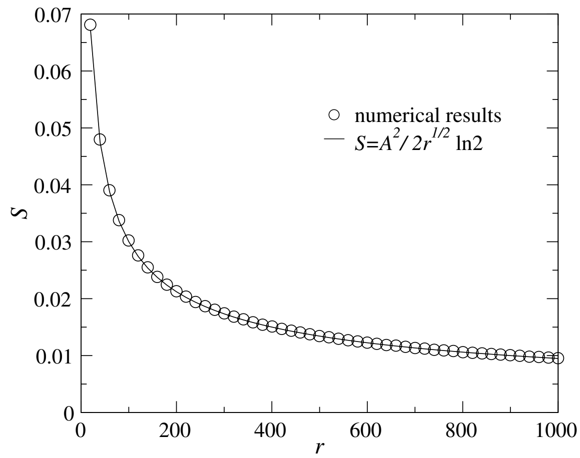

Figure 2. The correlation entropy as a function of the distance r (in units of $\sqrt{2}$ lattice constant) at the critical point.

Now let us analyze the critical behavior of the correlation entropy in detail. At the critical point, $S(\mathbf{i}) = 1$ because of $\langle\sigma_{\mathbf{i}}^z\rangle = 0$, and the correlation function behaves like

$$S_r \equiv \langle\sigma_{0,0}^z\sigma_{r,r}^z\rangle \simeq \frac{A}{r^{1/4}}, \tag{41}$$

where $A \simeq 0.645$. Then the two-site entropy can be simplified as

$$S(\mathbf{i}\cup\mathbf{j}) = 2 - \tfrac{1}{2}[(1+S_r)\log_2(1+S_r) + (1-S_r)\log_2(1-S_r)], \tag{42}$$

in the large-r limit. To the leading order, the correlation entropy scales like

$$S(0,0|r,r) = \frac{A^2}{2\ln 2}\frac{1}{r^{1/2}}, \tag{43}$$

as has been shown explicitly in figure 2. Around the critical point, the correlation entropy can be written as

$$S(\mathbf{i}|\mathbf{j}) \simeq \frac{1}{2\ln 2}\left(\langle\sigma_{\mathbf{i}}^z\sigma_{\mathbf{j}}^z\rangle^2 - \langle\sigma_{\mathbf{i}}^z\sigma_{\mathbf{j}}^z\rangle\langle\sigma_{\mathbf{i}}^z\rangle^2\right), \tag{44}$$

approximately. Taking the derivative, we then obtain

$$\frac{\partial S(\mathbf{i}|\mathbf{j})}{\partial T} = \frac{\langle\sigma_{\mathbf{i}}^z\sigma_{\mathbf{j}}^z\rangle - \langle\sigma_{\mathbf{i}}^z\rangle^2}{\ln 2}\frac{\partial\langle\sigma_{\mathbf{i}}^z\sigma_{\mathbf{j}}^z\rangle}{\partial T} - \frac{2\langle\sigma_{\mathbf{i}}^z\sigma_{\mathbf{j}}^z\rangle\langle\sigma_{\mathbf{i}}^z\rangle}{\ln 2}\frac{\partial\langle\sigma_{\mathbf{i}}^z\rangle}{\partial T}. \tag{45}$$

In the critical region below T_c, the dominant term in $\partial S(\mathbf{i}|\mathbf{j})/\partial T$ is $2\langle\sigma_{\mathbf{i}}^z\sigma_{\mathbf{j}}^z\rangle\langle\sigma_{\mathbf{i}}^z\rangle\partial\langle\sigma_{\mathbf{i}}\rangle/\partial T$, which leads to the fact that $\partial S(\mathbf{i}|\mathbf{j})/\partial T$ diverges as $T \to T_c$, and scales like

$$\frac{\partial S(\mathbf{i}|\mathbf{j})}{\partial T} \propto |T - T_c|^{-3/4}, \tag{46}$$

as we can see from figure 3(a). Then the critical exponent of $\partial S(\mathbf{i}|\mathbf{j})/\partial T$ below T_c is $\beta' = 3/4$, which is consistent with the critical exponent $1/8$ of $\langle\sigma_{\mathbf{i}}\rangle$, i.e.

$$\beta' = -\beta - (\beta - 1) = 1 - 2\beta. \tag{47}$$

While in the critical region above T_c, $\langle\sigma_{\mathbf{i}}^z\rangle$ vanishes and the dominating term in $S(\mathbf{i}|\mathbf{j})$ becomes the correlation function. Then $\partial S(\mathbf{i}|\mathbf{j})/\partial T$ scales like

$$\frac{\partial S(\mathbf{i}|\mathbf{j})}{\partial T} \propto \ln|T - T_c|, \tag{48}$$

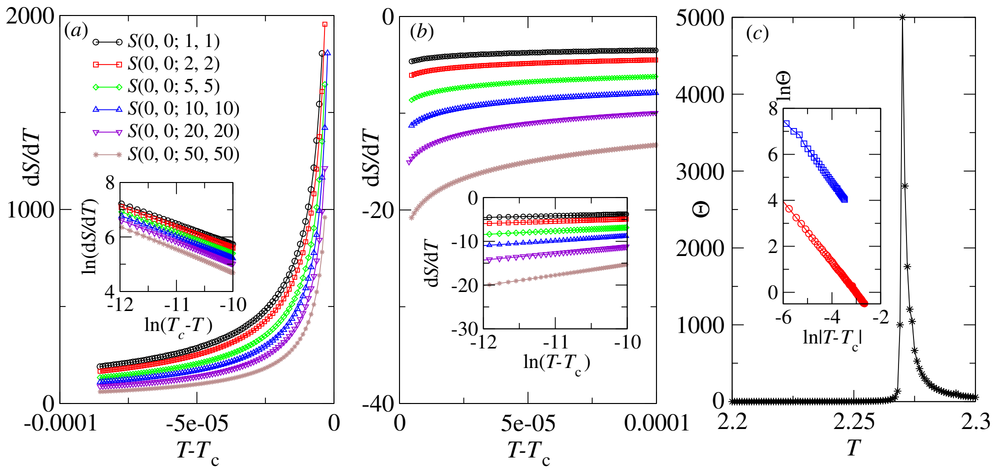

Figure 3. The critical behavior of the correlation entropy: (*a*) $\mathrm{d}S(0,0|N,N)/\mathrm{d}T$ below T_c, and the inset is to explore its critical exponent; (*b*) $\mathrm{d}S(0,0|N,N)/\mathrm{d}T$ above T_c; (*c*) Θ as a function of T around T_c, and the inset represents its rescaled behavior below (circle) and above (square) T_c.

which has the same critical behavior as the specific heat C_v, i.e.

$$\alpha = \alpha'. \tag{49}$$

Therefore, the critical exponent α' now becomes 0 (see figure 2(*b*)). Moreover, we also note that the slope of lines in the right inset of figure 2 is not the same. This is due to the fact that the exponent of the correlation function ν introduces the distance dependence in the $\partial S(\mathbf{i}|\mathbf{j})/\partial T$ above T_c.

In order to compute the exponent γ', let us first recall how to obtain the exponent γ for the susceptibility, which is defined by

$$\chi = \frac{1}{T}\sum_{m,n}\left[\left\langle\sigma_{0,0}^z\sigma_{m,n}^z\right\rangle - \langle\sigma_{0,0}\rangle^2\right]. \tag{50}$$

Here, the divergence of χ around the critical point arises from the two-dimensional integration on a power-law decay correlation function, i.e. equation (41) at infinite distance. That is

$$\chi \simeq \frac{2\pi}{T}\int_{r_0}^{\infty}\frac{f[r(T/T_c-1)]}{r^{1/4}} r\,\mathrm{d}r, \tag{51}$$

where r_0 is a cutoff which does not influence the divergence, and $f(r)$ is the interpolating function for the correlation function, which does not have contribution to the divergence. Then the susceptibility, in the rescaled length $t = |1 - T_c/T|r$, $t_0 = r_0|1 - T/T_c|$, becomes

$$\chi \simeq \frac{2\pi|1-T/T_c|^{-7/4}}{T}\int_{t_0}^{\infty} f[\mathrm{sgn}(T-T_c)t]t^{3/4}\,\mathrm{d}t. \tag{52}$$

Similarly, the integration of the correlation entropy takes the form

$$\begin{aligned}\Theta &\simeq 2\pi\int_{r_0}^{\infty}\frac{f^2[r(T/T_c-1)]}{r^{1/2}} r\,\mathrm{d}r,\\ &\simeq 2\pi|1-T/T_c|^{-3/2}\int_{t_0}^{\infty} f^2[\mathrm{sgn}(T-T_c)t]t^{1/2}\,\mathrm{d}t.\end{aligned} \tag{53}$$

Therefore, we have $\gamma' = 3/2$ (see figure 2(*c*)), and satisfy

$$\gamma' = 2\gamma - 2. \tag{54}$$

Finally, another scaling relation can be yielded from equations (47), (49) and (54):

$$\alpha' - \beta' + \gamma'/2 = 0. \tag{55}$$

This relation physically is the same as the standard scaling relation (38). The difference is that equation (55) comes from the critical behavior of a single quantity, i.e., the correlation entropy, while equation (38) depends on both the internal energy and the order parameter.

5. Quantum phase transition: the one-dimensional transverse-field Ising model

We now study the correlation entropy in the one-dimensional transverse-field Ising model whose Hamiltonian reads

$$H_{\text{Ising}} = -\sum_{j=1}^{N} \left[\lambda \sigma_j^x \sigma_{j+1}^x + \sigma_j^z\right], \qquad \sigma_1 = \sigma_{N+1}, \tag{56}$$

where λ is an Ising coupling in unit of the transverse-field. The Hamiltonian changes the number of down spins by two; the total space of the system then can be divided by the parity of spins. That is the Hamiltonian and the parity operator $P = \prod_j \sigma_j^z$ can be simultaneously diagonalized and the eigenvalues of P are ± 1. We confine our interests to the correlation entropy between two spins at positions i and j in the chain. Therefore, we need to consider both the single-site reduced density matrix ρ_i obtained from the ground-state wavefunction by tracing out all spins except that at site i, and the two-site reduced density matrix ρ_{ij} obtained by tracing out all spins except those at sites i and j. Then if there is no symmetry broken, such as in a finite-size system, according to the parity conservation, ρ_i has a diagonal form (31), and the reduced density matrix of two spins on a pair of lattice sites i and j can be put into the following block-diagonal form:

$$\rho_{ij} = \begin{pmatrix} u^+ & 0 & 0 & z^- \\ 0 & w_1 & z^+ & 0 \\ 0 & z^+ & w_2 & 0 \\ z^- & 0 & 0 & u^- \end{pmatrix} \tag{57}$$

in the basis $|\uparrow\uparrow\rangle, |\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle, |\downarrow\downarrow\rangle$. The elements in the density matrix ρ_{ij} can be calculated from the correlation function.

$$\begin{aligned} u^\pm &= \tfrac{1}{4}\left(1 \pm 2\langle\sigma_i^z\rangle + \langle\sigma_i^z\sigma_j^z\rangle\right), \\ w_1 &= w_2 = \tfrac{1}{4}\left(1 - \langle\sigma_i^z\sigma_j^z\rangle\right), \\ z^\pm &= \tfrac{1}{4}\left(\langle\sigma_i^x\sigma_j^x\rangle \pm \langle\sigma_i^y\sigma_j^y\rangle\right). \end{aligned} \tag{58}$$

Otherwise, if the symmetry is broken at the ground state of the ordered phase in the thermodynamic limit, i.e. $\langle\sigma^x\rangle \neq 0$, then the single-site reduced density matrix becomes

$$\rho_i = \frac{1}{2}\begin{pmatrix} 1 + \langle\sigma_i^z\rangle & \langle\sigma_i^x\rangle \\ \langle\sigma_i^x\rangle & 1 - \langle\sigma_i^z\rangle \end{pmatrix}, \tag{59}$$

and the two-site reduced density matrix returns to the original form (12) since no symmetry can be used to simply it. Therefore, the correlation entropy between the two sites i and j becomes

$$S(i|j) = 2\text{tr}(\rho_i \log_2 \rho_i) - \text{tr}(\rho_{ij} \log_2 \rho_{ij}). \tag{60}$$

Taking into account the translation invariance, the correlation entropy is simply a function of the distance between the two sites.

The transverse-field Ising model can be solved exactly in terms of Jordan–Wigner transformation. The mean magnetization is given by [28]

$$\langle\sigma^z\rangle = \frac{1}{N}\sum_{\phi}\frac{(1-\lambda\cos\phi)\tanh[\omega_\phi/T]}{\omega_\phi}, \tag{61}$$

where ω_ϕ is the dispersion relation,

$$\omega_\phi = \sqrt{1+\lambda^2-2\lambda\cos(\phi_q)}, \qquad \phi_q = 2\pi q/N, \tag{62}$$

where q is the integer (half-odd integer) for parity $P = -1(+1)$. The two-point correlation functions are calculated as [29]

$$\langle\sigma_0^x\sigma_r^x\rangle = \begin{vmatrix} a_{-1} & a_{-2} & \cdots & a_{-r} \\ a_0 & a_{-1} & \cdots & a_{-r+1} \\ \vdots & \vdots & \vdots & \vdots \\ a_{r-2} & a_{r-3} & \cdots & a_{-1} \end{vmatrix} \tag{63}$$

$$\langle\sigma_0^y\sigma_r^y\rangle = \begin{vmatrix} a_{1} & a_{0} & \cdots & a_{-r+2} \\ a_2 & a_{1} & \cdots & a_{-r+3} \\ \vdots & \vdots & \vdots & \vdots \\ a_{r} & a_{r-1} & \cdots & a_{1} \end{vmatrix} \tag{64}$$

$$\langle\sigma_0^z\sigma_r^z\rangle = \langle\sigma^z\rangle^2 - a_r a_{-r} \tag{65}$$

where

$$a_r = \frac{1}{N}\sum_{\phi}\frac{\cos(\phi r)(\lambda\cos\phi-1)\tanh[\omega_\phi/T]}{\omega_\phi} - \frac{\lambda}{N}\sum_{\phi}\frac{\sin(\phi r)\sin(\phi)\tanh[\omega_\phi/T]}{\omega_\phi}. \tag{66}$$

We show the correlation entropy $S(i|j)$ in the ground state as a function of coupling λ and distance between two sites $r = i - j$ in figure 4. The result is also impressive. As is well known [17], the ground state of the transverse-field Ising model consists of two different phases, whose corresponding physical picture can be understood from both weak and strong coupling limits. If $\lambda \to 0$, all spins are polarized along the z-direction, the ground state then is a paramagnet and in the absence of long-range correlation, while in the limit $\lambda \gg 1$, the strong Ising coupling introduces magnetic long-range correlation in the order parameter σ^x to the ground state. The competition between these two different orders leads to a quantum phase transition at the critical point $\lambda_c = 1$. From figure 4, we can see that the correlation entropy tends to zero quickly as the distance between two sites increases in the paramagnetic phase. These phenomena can be well understood from the fact that the ground state in this phase is non-degenerate and almost fully polarized; therefore, knowledge of the state at one site i does not effect the state of another site j far away, which leads to zero information in common between two sites. However, this scene is not true in another phase. When $\lambda > 1$, the ground state is twofold degenerate and possesses a long-range correlation. Before the measurement, the uncertainty of the state at an arbitrary site is very large. However, if we learn the state of one site, the state at another site, even far away, is almost determined which leads to a finite correlation entropy between two sites even if they are separated far away from each other.

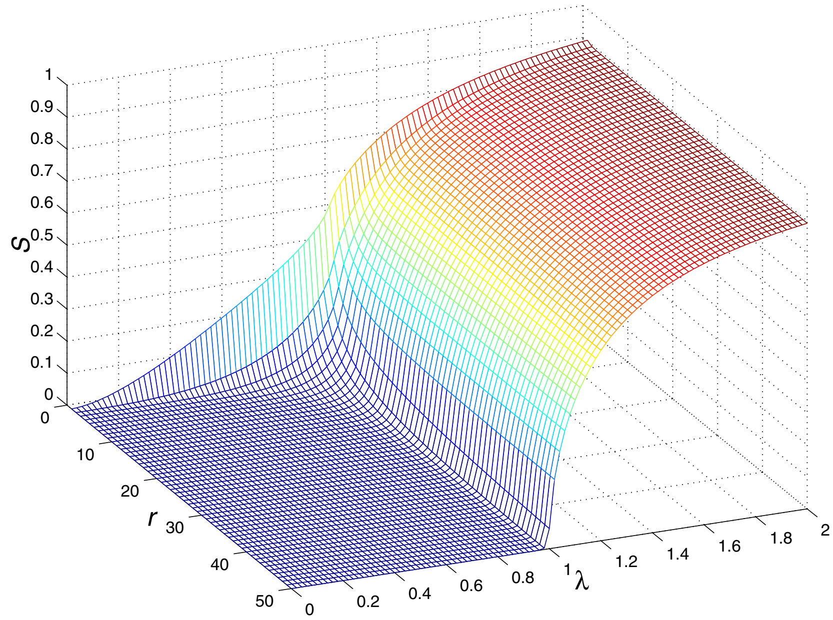

Figure 4. The correlation entropy as a function of λ and the distance r (in unit of lattice constant) at $T = 0$ for a system with $N = 5000$.

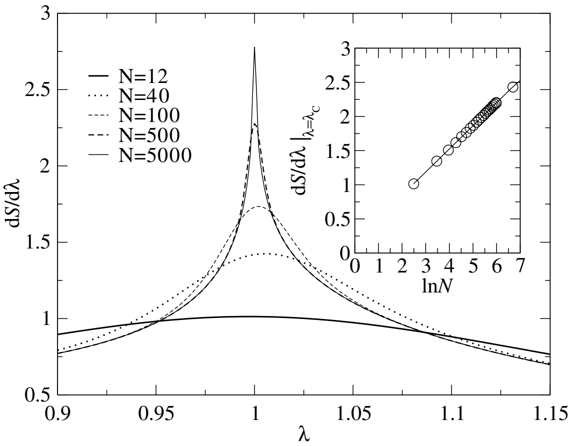

Figure 5. The scaling behavior the correlation entropy between two neighboring sites.

Obviously, the behavior of the correlation entropy in the transverse-field Ising model is quite different from the quantum entanglement. In the previous works [10, 11] on the pairwise entanglement in the ground state of this model, it has been shown that the concurrence vanishes unless the two sites are at most next-nearest neighbors. In the paramagnetic phase, the correlation entropy shares similar properties in common with the concurrence. In the ordered phase, however, the correlation entropy does not vanish even the distance between the two sites becomes very large, such as 50 lattice constant. Moreover, the correlation entropy also shows interesting scaling behavior, just as that of the concurrence, around the critical point, as is shown in figure 5. Moreover, we find that at the critical point the first derivative of

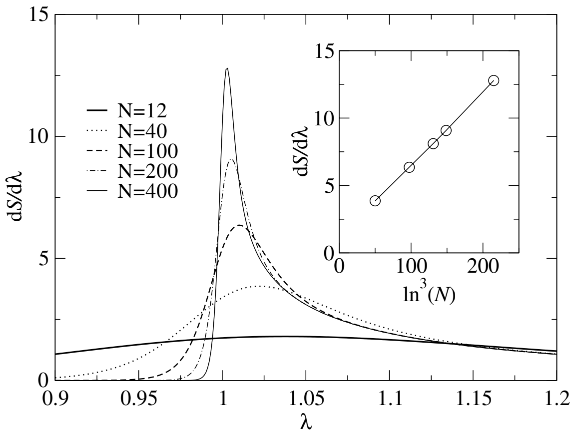

Figure 6. The scaling behavior the correlation entropy between two sites at the longest distance.

the correlation entropy between two neighboring sites scales like

$$\left.\frac{\mathrm{d}S(0|1)}{\mathrm{d}\lambda}\right|_{\lambda=\lambda_c} \simeq \text{const.} \times \ln N. \tag{67}$$

or

$$S(0|1) \simeq S(0|1)|_{\lambda=\lambda_c} + \text{const.} \times (\lambda - \lambda_c) \ln N. \tag{68}$$

However, for those sites are separated far away, the correlation entropy shows a quite different scaling behavior. For example, in figure 6, we show the scaling behavior the correlation entropy between the two sites at the longest distance in a ring. This first observation is that when $N \to \infty$, $\mathrm{d}S(0|N/2)/\mathrm{d}\lambda$ becomes divergent. Moreover, detailed analysis reveals that the maximum value of the first derivative of the correlation entropy between two farthest sites in a ring scales like

$$\frac{\mathrm{d}S(0|N/2)}{\mathrm{d}\lambda} \simeq \text{const.} \times \ln^3 N. \tag{69}$$

which differs from $\ln N$ for $\mathrm{d}S(0|1)/\mathrm{d}\lambda$. Obviously, these interesting scaling behaviors enable us to learn the physics of real infinite system from the scaling analysis. Based on the scaling ansatz, the correlation entropy, considered as a function of system size and the coupling, is a function of $N^{1/\nu}(\lambda - \lambda_m)$. In the case of logarithmic divergence, the correlation entropy behaves as $\mathrm{d}S/\mathrm{d}\lambda - \mathrm{d}S/\mathrm{d}\lambda|_{\lambda=\lambda_m} \sim Q[N^{1/\nu}(\lambda - \lambda_m)]$, where $Q(x) \propto \ln x$ for large x. In figures 7 and 8, we perform the scaling analysis and find that both $S(0|1)$ and $S(0|N/2)$ can be collapsed to a single curve for $\nu = 1$ and $\nu = 4/5$, respectively.

On the other hand, there is no thermal phase transition in the one-dimensional quantum spin system according to the Mermin–Wagner theorem [30]. Thus let us study the properties of the correlation entropy away from zero temperature. The results are shown in figures 9 and 10 for $T = 0.2$ and 0.5, respectively. We can see that at lower temperature $T = 0.2$, the correlation entropy is broken only around the critical region $\lambda \sim 1$. As the temperature increases, the correlation entropy in larger λ region vanishes. These observations tell us that the correlation entropy is a decreasing function of the temperature, as we can see from figure 11. Since the broken symmetry only exists in the ground state of an infinite system and the thermal fluctuation tends to decrease the correlation entropy, it is not possible to reestablish such a long-range correlation at finite temperatures. Therefore, no thermal phase transition

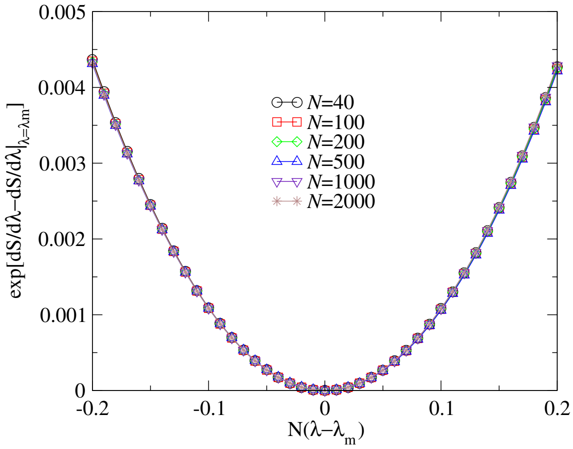

Figure 7. The finite-size scaling analysis for the case of logarithmic divergence. The correlation entropy between the two neighboring sites, considered as a function of system size and the coupling, collapses on a single curve for various system sizes.

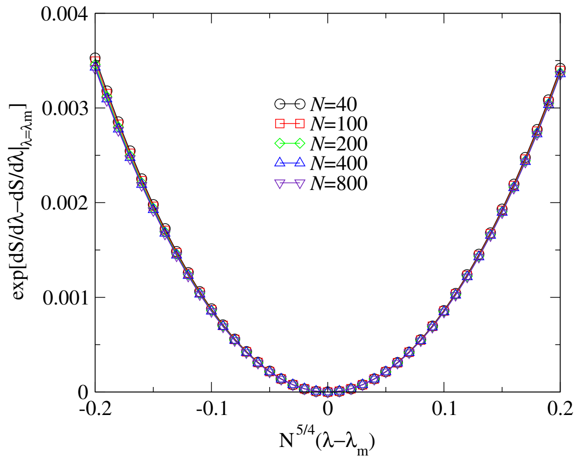

Figure 8. The finite-size scaling analysis for the case of logarithmic divergence. The correlation entropy between two sites at the longest distance, considered as a function of system size and the coupling, collapses on a single curve for various system sizes.

happens in the one-dimensional transverse-field Ising model. This observation, based on the numerical calculation, is consistent with the Mermin–Wagner theorem [30].

6. Discussions and prospects

With analytical studies and numerical calculations, we have discovered the rigorous relation between the correlation entropy and the long-range correlation. The relation strongly indicates us the non-trivial role played by the correlation entropy in the critical phenomena. This discovery motivates us to study both the thermal and the quantum phase transitions from the point of view of information theory, i.e. mutual information, whose non-vanishing behavior at long distance really witnesses the violation of the extensive properties of the entropy in

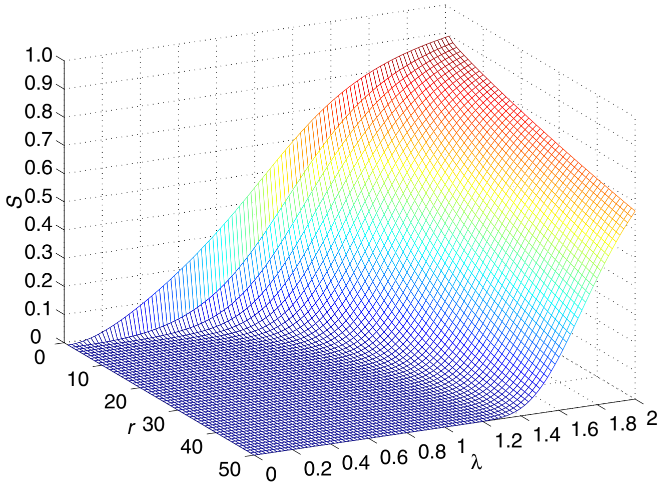

Figure 9. The correlation entropy as a function of λ and the distance r (in unit of lattice constant) at $T = 0.2$. Obviously, at low temperature, the correlation entropy at long distance vanishes in the quantum critical region around $\lambda = 1$.

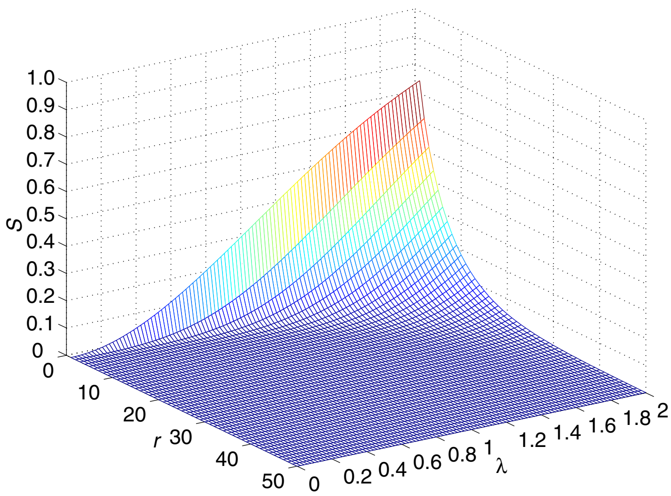

Figure 10. The correlation entropy as a function of λ and the distance r (in unit of lattice constant) at $T = 0.5$. At higher temperature, the correlation entropy vanishes at long distance.

the statistical physics, i.e. $S(\mathrm{A} \cup \mathrm{B}) = S(\mathrm{A}) + S(\mathrm{B})$. In the two models we studied in this paper, since the correlation length at the critical point diverges, the physics of the system has a strong dependence on the system size, i.e., the scaling behavior. This observation implies that the entropy at the critical point is no longer a linear function of the volume of the system, i.e. $S \neq sV$. In the one-dimensional system, it has already been noted that the entropy of the subsystem satisfies $S(x) \propto \ln(x)$ [32], where x is the length of the subsystem in the critical region of some spin systems. Then, from this point of view, the spatial degree of freedom of the system is reduced around the critical point.

On the other hand, though we restrict ourselves to the two-point correlation entropy in the above studies, if the system processes a block–block order, such as a dimer order [31], it may

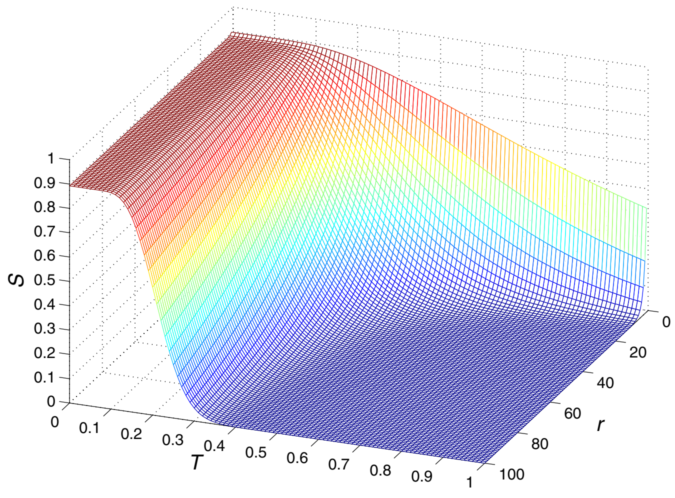

Figure 11. The correlation entropy as a function of temperature T and the distance r (in unit of lattice constant) at $\lambda = 2.0$. We can see from the figure that the correlation entropy is protected by an energy gap at low temperature.

be useful to investigate the properties of block–block correlation entropy. A simple example is the Majumdar–Ghosh model with the Hamiltonian

$$H = \sum_i (J_1\sigma_i \cdot \sigma_{i+1} + J_2\sigma_i \cdot \sigma_{i+2}), \tag{70}$$

where J_2 is the coupling between the two next-nearest neighbor sites. In this model, if $J_2 = 1/2$, the ground state is a uniformly weighted superposition of the two nearest-neighbor valence bond states [31]

$$\begin{aligned} |\psi_1\rangle &= [1, 2][3, 4] \cdots [L-1, L] \\ |\psi_2\rangle &= [L, 1][2, 3] \cdots [L-2, L-1] \end{aligned} \tag{71}$$

where

$$[i, j] = \frac{1}{\sqrt{2}}(|\uparrow\rangle_i|\downarrow\rangle_j - |\downarrow\rangle_i|\uparrow\rangle_j). \tag{72}$$

Then the block–block correlation entropy can help us to understand such a dimer order.

Moreover, from the definition of the correlation entropy, it is also useful to introduce a characteristic length for the statistical system, below which the extensive properties of the entropy are violated. Such a characteristic length has a non-trivial meaning, since the extensive property of the entropy in the statistical physics is only valid above this scale. A simple example is the molecule which is composed of some atoms. When we study the physics of molecule gas, we have to regard a molecule as a whole because of its internal order. Only when the temperature is high enough to break its order, does the atom then play the important role to the statistical properties of the system.

Though we verify the non-trivial behavior of the correlation entropy in terms of spin systems, the rigorous relation between the non-vanishing correlation entropy and the long-range correlation is valid for all many-body systems. Therefore, it is expected to provide more physical intuition into the critical phenomena, such as Bose–Einstein condensation and superconductivity from the point of view of the correlation entropy. Take the former as a simple example, the reduced density matrix between the two locations in the spacetime can be expressed in terms of bosons operators $a^\dagger_{\mathbf{x},\mathbf{p}}|0\rangle = \exp(-\mathrm{i}\mathbf{px})$ in space representation. At high temperatures, $\langle \mathbf{p}|\rho_{\mathbf{xx}'}|\mathbf{p}'\rangle$ vanishes as $\mathbf{x}-\mathbf{x}'$ increases. Only when the condensation happens, $\langle \mathbf{0}|\rho_{\mathbf{xx}'}|\mathbf{0}\rangle$ leads to a non-vanishing correlation entropy, just as what we have shown for the correlation entropy in quantum spin systems.

7. Summary

In summary, the correlation entropy plays a universal role in understanding critical phenomena. Its non-vanishing behavior not only helps us have deep understanding to the entropy in the statistical physics but also sheds light on the long-range correlation in the critical behavior.

Acknowledgments

This work is supported by the Earmarked Grant for Research from the Research Grants Council of HKSAR, China (project no. CUHK N_CUHK204/05 and CUHK 400807), and NSFC grants. We thank XG Wen for helpful discussions.

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