# Quantum Correlations in Spin Chains at Finite Temperatures and Quantum Phase Transitions

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We compute the quantum correlation [quantum discord (QD)] and the entanglement (EOF) between nearest-neighbor qubits (spin-1/2) in an infinite chain described by the Heisenberg model ($XXZ$ Hamiltonian) at finite temperatures. The chain is in the thermodynamic limit and thermalized with a reservoir at temperature $T$ (canonical ensemble). We show that QD, in contrast to EOF and other thermodynamic quantities, spotlight the critical points associated with quantum phase transitions (QPT) for this model even at finite $T$. This remarkable property of QD may have important implications for experimental characterization of QPTs when one is unable to reach temperatures below which a QPT can be seen.

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Quantum phase transition (QPT) is a purely quantum process [1] occurring at absolute zero temperature ($T = 0$), where no thermal fluctuations exist and hence no classical phase transition is allowed to occur. QPT is caused by changing the system's Hamiltonian, such as an external magnetic field or the coupling constant. These quantities are generally known as the tuning parameter. As one changes the Hamiltonian one may reach a special point (critical point) where the ground state of the system suffers an abrupt change mapped to a macroscopic change in the system's properties. This change of phase is solely due to quantum fluctuations, which exist at $T = 0$ due to the Heisenberg uncertainty principle. This whole process is called QPT. The paramagnetic-ferromagnetic transition in some metals [2], the superconductor-insulator transition [3], and superfluid-Mott insulator transition [4] are remarkable examples of this sort of phase transition.

In principle QPTs occur at $T = 0$, which is unattainable experimentally due to the third law of thermodynamics. Hence, one must work at very small $T$, as close as possible to the absolute zero, in order to detect a QPT. More precisely, one needs to work at regimes in which thermal fluctuations are insufficient to drive the system from its ground to excited states. In this scenario quantum fluctuations dominate and one is able to measure a QPT.

So far the theoretical tools available to determine the critical points (CP) for a given Hamiltonian assume $T = 0$. For spin chains, for instance, the CPs are determined studying, as one varies the tuning parameter, the behavior of either its magnetization, or bipartite [5] and multipartite [6] entanglement, or its quantum correlation (QC) [7]. By investigating the extremal values of these quantities as well as the behavior of their first and second order derivatives one is able to spotlight the CP. However, the $T = 0$ assumption limits a direct connection between these theoretical "CP detectors" and experiment. Indeed, if thermal fluctuations are not small enough excited states become relevant and the tools developed so far cannot be employed to clearly indicate the CP.

In this Letter we remove this limitation and present a theoretical tool that is able to clearly detect CPs for QPTs at finite $T$. We show that the behavior of strictly QCs [8] at finite $T$, as given by the thermal quantum discord (TQD) [9], unambiguously detects CPs for QPTs that could only be seen, using previous methods, at $T = 0$ [7]. This remarkable property of TQD, on one hand, is an important tool that can be readily applied to reduce the experimental demands to determine CPs for QPTs, or even allow such a detection for those systems where today's technology makes it virtually impossible to achieve the necessary $T$ below which quantum fluctuations dominate. One the other hand, this characteristic of TQD shows that QPTs have a decisive influence on a system's physical property not only for small $T$ but also above $T$ where quantum fluctuations no longer dominate.

In order to show that TQD detects a QPT at finite $T$, we study the anisotropic spin-1/2 Heisenberg chain ($XXZ$) in the thermodynamic limit. We assume the infinite chain to be in thermal equilibrium with a reservoir at temperature $T$; i.e., its density matrix is described by the canonical ensemble. Tracing out all spins but the two nearest neighbors we get their reduced density matrix as a function of two-point correlation functions, which are evaluated by solving a set of nonlinear integral equations (NLIE) [10,11]. The two-qubit density matrix allows us to compute TQD and investigate its properties for $T > 0$ as we change the system's Hamiltonian. We show that TQD is maximal and its first-order derivative with respect to the tuning parameter is discontinuous at the quantum CP, not only at $T = 0$ [7], but also at $T > 0$. This behavior is robust enough to be seen for high $T$. Furthermore, we have also computed the entropy, magnetization, magnetic susceptibility, and specific heat, for the whole chain, and two-site correlations between the two nearest-neighbor spins as well as their entanglement. We show that none of these quantities detect unambiguously the CP for $T > 0$. We also discuss why TQD possesses such a unique behavior in contrast to another quantity, namely, the entanglement between the two nearest neighbors.

The $XXZ$ Hamiltonian can be written as

$$H = J\sum_{j=1}^{L}(\sigma_j^x\sigma_{j+1}^x + \sigma_j^y\sigma_{j+1}^y + \Delta\sigma_j^z\sigma_{j+1}^z), \qquad (1)$$

where periodic boundary conditions are assumed and $\Delta$ is the anisotropy parameter. Here $L \to \infty$ and $\sigma_j^x$, $\sigma_j^y$, and $\sigma_j^z$ are the usual Pauli matrices acting on the $j$-th qubit. Throughout this Letter $\hbar = 1$ and $J = 1$ unless noted otherwise. At $T = 0$ the $XXZ$ model has two CPs [12]. At $\Delta = 1$ we have a continuous phase transition and at $\Delta = -1$ we have a first-order transition.

The density matrix for a system in equilibrium with a thermal reservoir is $\rho = \exp(-\beta H)/Z$, where $\beta = 1/kT$, $Z = \mathrm{Tr}\{\exp(-\beta H)\}$ is the partition function, and the Boltzmann's constant $k$ is set to unity. The nearest-neighbor two-qubit state is obtained by tracing all but the first two spins, $\rho_{12} = \mathrm{Tr}_{L-2}\{\rho\}$. Because of the translation invariance and $U(1)$ invariance ($[H, \sum_{j=1}^{L}\sigma_j^z] = 0$) of (1), we can write the reduced density matrix as follows,

$$\rho_{12} = \begin{pmatrix} \frac{1+\langle\sigma_1^z\sigma_2^z\rangle}{4} & 0 & 0 & 0 \\ 0 & \frac{1-\langle\sigma_1^z\sigma_2^z\rangle}{4} & \frac{\langle\sigma_1^x\sigma_2^x\rangle}{2} & 0 \\ 0 & \frac{\langle\sigma_1^x\sigma_2^x\rangle}{2} & \frac{1-\langle\sigma_1^z\sigma_2^z\rangle}{4} & 0 \\ 0 & 0 & 0 & \frac{1+\langle\sigma_1^z\sigma_2^z\rangle}{4} \end{pmatrix}. \qquad (2)$$

These two-point correlation functions can be written in its simplest form in terms of derivatives of the free energy $f = (-1/\beta)\lim_{L\to\infty}(\ln Z)/L$,

$$\langle\sigma_j^z\sigma_{j+1}^z\rangle = \partial_\Delta f/J, \qquad \langle\sigma_j^x\sigma_{j+1}^x\rangle = (u - \Delta\partial_\Delta f)/2J, \qquad (3)$$

with $u = \partial_\beta(\beta f)$ the internal energy. In order to determine the free energy in the thermodynamic limit and at finite $T$ one has to solve a suitable set of NLIE [10,11,13].

Now we can use (2) in order to show that the entanglement, as measured by the entanglement of formation (EOF) [14], is $\mathrm{EoF} = -g(f(C)) - g(1 - f(C))$, with $f(C) = (1 + \sqrt{1 - C^2})/2$, $g(f) = f\log_2(f)$, and

$$C = \mathrm{Max}\{0, |\langle\sigma_1^x\sigma_2^x\rangle| - |1 + \langle\sigma_1^z\sigma_2^z\rangle|/2\} \qquad (4)$$

the concurrence, an entanglement monotone. EOF quantifies a class of QCs that cannot be created by local operations and classical communication (LOCC) only [15]. Recently, however, it became clear that there exist more general QCs if one removes the LOCC restriction. These correlations are measured by the quantum discord (QD) [8] and it is believed that QD quantifies all correlations between two systems that has a pure quantum origin. Note that EOF and QD coincide for bipartite pure states; for mixed states, though, their difference becomes manifest being both zero, however, when only classical correlations are present. We can also conceptually understand QCs in comparison with entanglement by noting that the latter is due to the superposition principle applied to the whole Hilbert space of a bipartite system. However, QCs as given by QD captures, on top of that, the correlations coming from superposition of states within each subsystem, a purely quantum effect that it is not possible classically [16]. From this perspective, one can better grasp why there exist states with zero entanglement but finite QCs [17]. Another interesting and operational interpretation for QD is achieved looking at the thermodynamic properties of a quantum system. In [18] it is shown that QD is related to the difference of work that can be extracted acting either globally or locally at a heat bath with a bipartite state when one-way communication is allowed.

For state (2) QD is [19] $\mathrm{QD} = [g(1 - 2d_x - d_z) + 2g(1 + d_z) + g(1 + 2d_x - d_z)]/4 - [g(1 + D) + g(1 - D)]/2$, with $d_x = \langle\sigma_1^x\sigma_2^x\rangle$, $d_z = \langle\sigma_1^z\sigma_2^z\rangle$, and

$$D = \mathrm{Max}\{|\langle\sigma_1^x\sigma_2^x\rangle|, |\langle\sigma_1^z\sigma_2^z\rangle|\}. \qquad (5)$$

Note that either $|\langle\sigma_1^x\sigma_2^x\rangle|$ or $|\langle\sigma_1^z\sigma_2^z\rangle|$ is responsible for the value of $D$. As will be seen, it is the interplay between these two correlations that is relevant in our understanding of why QD detects a QPT at finite $T$ and EOF does not [20].

We are now in a position to present the behavior of TQD and EOF between two nearest-neighbor qubits in an infinite spin chain at finite $T$. We first plot TQD and EOF, for several $T$, as a function of the tuning parameter $\Delta$. This allows us to prove the main claim in this Letter, namely, that TQD detects a CP of a QPT at finite $T$ while EOF does not. Looking at Fig. 1 we see that EOF is maximal in the

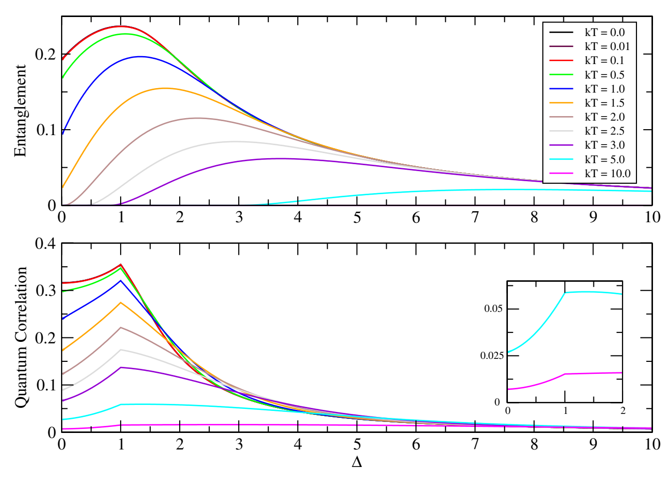


FIG. 1 (color online). EOF (top) and QD (bottom) as functions of the tuning parameter $\Delta$ for the $XXZ$ model in the thermodynamic limit. The inset depicts QD for high $T$ near the CP. $T$ increases from top to bottom. The curves for $T = 0$ and $T = 0.01$ cannot be distinguished from the $T = 0.1$. Here and in the following graphics all quantities are dimensionless.

CP $\Delta = 1$ only at $T = 0$, agreeing with the results of [7]. As we increase $T$ the maximum no longer occurs at $\Delta = 1$, moving to the region where $\Delta > 1$. Also, the higher $T$ the farther from the CP is located the maximum of EOF. On the other hand, TQD is maximal at $\Delta = 1$ when $T = 0$ and does not appreciably move away for $T \leq 3$. Moreover, its first-order derivative is discontinuous at the CP not only at $T = 0$ but also at $T > 0$, a remarkable result showing that TQD inherits at $T > 0$ all of its important properties previously seen only at $T = 0$. This discontinuity of the first derivative of TQD at $\Delta = 1$ is our CP detector for non-null $T$. In order to prove this unique behavior of TQD, we have computed for several $T$ many thermodynamic quantities for the infinite spin chain and also the pairwise correlations as a function of the tuning parameter $\Delta$. As can be seen in Fig. 2, none of these quantities can clearly detect the CP at $T > 0$.

Because of subtleties of the NLIE at $\Delta = -1$ ($J > 0$), it is convenient to investigate how TQD behaves near the CP $\Delta = -1$ by means of numerical diagonalization of the Hamiltonian (1) [22]. We computed its thermal density matrix, and then calculated the nearest-neighbor reduced density matrix for lattice sizes $L = 8$ and 10. Again, only TQD was able to detect the CP for $T > 0$. Looking at Fig. 3 we clearly see that TQD successfully picks the CPs at $\Delta = \pm 1$ while EOF does not. For finite $T$, the first derivative of TQD is discontinuous at both CPs. EOF, on the other hand, is zero around $\Delta = -1$ and its maximum gets shifted to the right at $\Delta = 1$. Note that for small $T$ and $\Delta = -1$ TQD also resembles its behavior at $T = 0$, namely, being discontinuous at the CP [7].

In order to complement our results, we fix the anisotropy parameter at $\Delta = 1$ and then vary the coupling constant $J$ from negative to positive values, i.e., we go from a ferromagnetic to an antiferromagnetic regime. As can be seen in Fig. 4 TQD decreases as one varies $J$ towards zero from both sides [9]. Similar to the previous case, TQD inherits for finite $T$ its behavior at $T = 0$. However, EOF is only nonzero for the antiferromagnetic regime; and for finite $T$ this only occurs away from the vicinity of $J = 0$. In other words, the behavior of TQD around $J = 0$ and $T > 0$ are qualitatively similar to its behavior at $T = 0$ while this is no longer true for the behavior of EOF.

We can understand this unique aspect of TQD, especially in contrast to EOF, by taking a careful look at the analytical expressions giving EOF and TQD. The main difference in behavior between EOF and TQD is connected to Eqs. (4) and (5), being directly related to the maximization process leading to these quantities. For the $XXZ$ model and at finite $T$, one can show that around the two CPs the function maximizing (4) does not abruptly change. It is either 0 or $|\langle\sigma_1^x\sigma_2^x\rangle| - |1 + \langle\sigma_1^z\sigma_2^z\rangle|/2$. On the other hand, for (5), the function maximizing it changes exactly at the CPs. Before the CPs one has either $|\langle\sigma_1^z\sigma_2^z\rangle|$ or $|\langle\sigma_1^x\sigma_2^x\rangle|$ as the maximum but after them this role is exchanged. Indeed, in the vicinity of $\Delta < -1$ $D$ is given by $|\langle\sigma_1^z\sigma_2^z\rangle|$ while for $-1 < \Delta < 1$ it is determined by $|\langle\sigma_1^x\sigma_2^x\rangle|$ (see Fig. 2). Finally, in the vicinity of $\Delta > 1$ it is determined by $|\langle\sigma_1^z\sigma_2^z\rangle|$. It is this change in the function maximizing $D$, which occurs at $T = 0$ [7] and shown here also to occur at $T > 0$, that is responsible for the discontinuity of the first derivate of TQD. For the $XXX$ model, $|\langle\sigma_1^x\sigma_2^x\rangle| = |\langle\sigma_1^z\sigma_2^z\rangle|$, and therefore no cusplike behavior for TQD is observed. However, TQD is only zero at $J = 0$ for any $T$ while EOF is always zero in the vicinity of $J = 0$ for $T > 0$. Moreover, working with small chains (up to 10 qubits) for various $T$, we observed that the second derivative of TQD possesses a relatively high value near $J = 0$. We believe that it is likely that as one approaches the thermo-

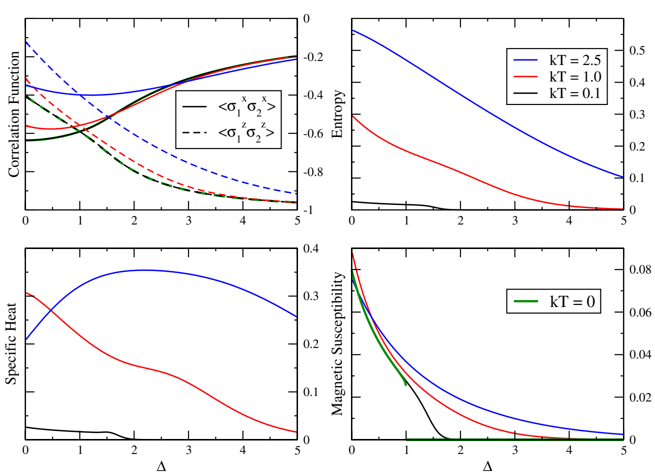


FIG. 2 (color online). Thermodynamic quantities for the $XXZ$ model in the thermodynamic limit. The $T = 0$ and $T = 0.1$ curves for the two-point correlation functions are indistinguishable. Note that at $T = 0$ the magnetic susceptibility also detects the phase transition being discontinuous at the CP [25]. The specific heat and entropy are null at $T = 0$.

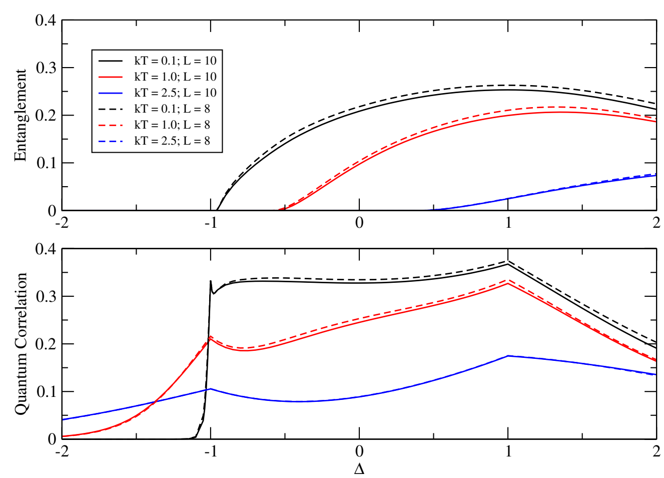


FIG. 3 (color online). EOF and QD for a chain of 8 and 10 qubits described by the $XXZ$ model. QD detects both quantum critical points at finite $T$ while EOF does not.

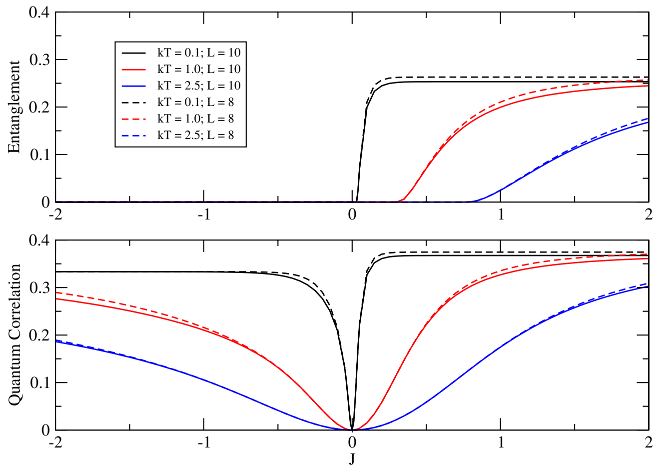


FIG. 4 (color online). EOF and QD for a chain of 8 and 10 qubits described by the $XXX$ model.

dynamic limit the peak of the second derivative moves towards $J = 0$.

In summary, we presented a remarkable characteristic of quantum correlations as given by the quantum discord: its ability to detect critical points of quantum phase transitions at finite $T$. Indeed, by solving an infinite chain described by the $XXZ$ model in the thermodynamic limit, we showed that QD is able to highlight the CPs of QPTs for $T > 0$ while neither the entanglement nor any thermodynamic quantity achieve the same feat. This property of QD may be useful in the experimental detection of CPs for QPTs where one is not able to reach the temperatures below which a QPT can be seen. Conceptually, this capacity of QD to detect CPs of QPTs for $T > 0$ and its interesting and puzzling dynamical robustness against noise [23,24] illustrate the broad range of scenarios where QD helps in the understanding of fundamental issues of quantum mechanics.

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