Quantum and classical thermal correlations in the XY spin-$\frac{1}{2}$ chain

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We investigate pairwise quantum correlation as measured by the quantum discord as well as its classical counterpart in the thermodynamic limit of anisotropic XY spin-$1/2$ chains in a transverse magnetic field for both zero and finite temperatures. Analytical expressions for both classical and quantum correlations are obtained for spin pairs at any distance. In the case of zero temperature, it is shown that the quantum discord for spin pairs farther than second neighbors is able to characterize a quantum phase transition, even though pairwise entanglement is absent for such distances. For finite temperatures, we show that quantum correlations can be increased with temperature in the presence of a magnetic field. Moreover, in the XX limit, thermal quantum discord is found to be dominant over classical correlation while the opposite scenario takes place for the transverse field Ising model limit.

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I. INTRODUCTION

Since its conception, quantum mechanics has been extensively applied to condensed matter systems [1]. This endeavor resulted in important conceptual and technological advances. In the past few decades, this scenario has gained even more strength with the birth of quantum-information science (QIS) [2]. In this context, quantum spin systems have played a central role in several applications for both quantum communication [3] and quantum computation [4]. Indeed, quantum spin models describe the effective interactions in a variety of physical systems [5], for example, quantum Hall systems, high-temperature superconductors, heavy fermions, and magnetic compounds. More generally, low-dimensional systems such as those described by interacting spins are particularly interesting because of the presence of typically pronounced quantum fluctuations as well as the possibility of their realization by several distinct physical approaches [6,7].

A key concept in QIS is the quantum correlation among parts of a composite quantum system, which is a fundamental resource for several applications in quantum information [2]. The existence of quantum correlations were first noted in nonseparable (i.e., entangled) states. Entanglement was pointed out by Schrödinger in 1935 [8] as the characteristic trait of quantum mechanics. Since then, entanglement has been basically the only kind of quantum correlation theoretically and experimentally explored. However, in the past few years, it has been realized that there exist nonclassical correlations which are not captured by entanglement measures [9,10]. In general, a quantum correlation, which can be measured by the *quantum discord* (QD) [9], often arises as a consequence of coherence between different partitions in a quantum system, being present even in separable states. Recently, QD was analyzed in a number of contexts, for example, low-dimensional spin models [11–15], open quantum systems [16–19], biological [20], and relativistic [21] systems. Moreover, there exist strong indications that the QD is the resource responsible for the speed up in the model of computation known as deterministic quantum computation with one quantum bit [22,23].

In this article we consider pairwise QD in an infinite anisotropic XY spin-$1/2$ chain in the presence of an external transverse magnetic field for both zero and finite temperatures. Our aim is to explore, in the thermodynamical regime, the behavior of QD for spin pairs arbitrarily distant and also take into account the effect of temperature on the behavior of correlations. Such contributions, which have not been considered in previous works, will be shown to bring several new effects to the subject. In particular, as we will show, the QD for spin pairs more distant than second neighbors is able to characterize a quantum phase transition (QPT). This is a remarkable behavior, since a signature of the QPT can be available through the QD even for distances where pairwise entanglement is absent. Moreover, we will show that the QD may increases with both temperature and magnetic field for certain regions of parameter space. This result will extend, to the thermodynamic limit, the previous analysis for two-spin Hamiltonians reported in Ref. [13]. Finally, we will discuss the dominance of quantum correlation over classical correlation for different limits of the XY model, showing that the QD is greater than its classical counterpart for the isotropic limit (XX model), with the opposite scenario taking place for the transverse field Ising model. These results generalize those of Refs. [11] and [12].

II. CORRELATIONS IN BIPARTITE QUANTUM SYSTEMS

The information-theoretical measure of the total correlation between the partitions of a bipartite quantum state ρ_{AB} is the quantum mutual information [24,25]

$$I(\rho_{AB}) = S(\rho_A) + S(\rho_B) - S(\rho_{AB}), \tag{1}$$

where $S(\rho) = -\mathrm{Tr}\rho \log_2 \rho$ is the von Neumann entropy and ρ_A (ρ_B) is the reduced-density operator of the partition A (B). The nonclassical correlation present in ρ_{AB} can be quantified by the quantum discord, which is defined as [9]

$$D(\rho_{AB}) \equiv I(\rho_{AB}) - C(\rho_{AB}), \tag{2}$$

where

$$C(\rho_{AB}) \equiv S(\rho_A) - \min_{\{\Pi_j\}} S_{\{\Pi_j\}}(\rho_{A|B}) \tag{3}$$

is the classical correlation present in the composite state ρ_{AB} [26]. In Eq. (3), the conditional entropy $S_{\{\Pi_j\}}(\rho_{A|B})$ can be defined as

$$S_{\{\Pi_j\}}(\rho_{A|B}) = \sum_j q_j S(\rho_A^j), \tag{4}$$

with $q_j = \mathrm{Tr}\,[(\mathbf{1}_A \otimes \Pi_j)\rho_{AB}(\mathbf{1}_A \otimes \Pi_j)]$ and $\rho_A^j = \mathrm{Tr}_B[(\mathbf{1}_A \otimes \Pi_j)\rho_{AB}(\mathbf{1}_A \otimes \Pi_j)]/q_j$. The minimum in Eq. (3) is taken over a complete set of projective measures $\{\Pi_j\}$ on the partition B. For pure states, we have that both quantum and classical correlations are equal to entanglement entropy [24,26]. On the other hand, for mixed states, entanglement is only a part of this nonclassical correlation [9,22,23].

In order to compare our results for the QD with those for pairwise entanglement, we will use the entanglement of formation as a measure of entanglement. The concurrence (c) is monotonically related to the entanglement of formation by the following expression:

$$\mathcal{E}(\rho_{AB}) = \mathcal{H}_{\mathrm{bin}}\{[1 + \sqrt{1 - [c(\rho_{AB})]^2}]/2\},$$

where $\mathcal{H}_{\mathrm{bin}}(x) = -x\log_2 x - (1-x)\log_2(1-x)$ is the binary entropy. For two qubits the concurrence reduces to the simple form [27]

$$c(\rho_{AB}) = \max(0, \sqrt{\lambda_1} - \sqrt{\lambda_2} - \sqrt{\lambda_3} - \sqrt{\lambda_4}), \tag{5}$$

where λ_i $(i = 1,2,3,4)$ are the eigenvalues of $\rho_{AB}\tilde{\rho}_{AB}$ in decreasing order, $\tilde{\rho}_{AB} = (\sigma_A^y \otimes \sigma_B^y)\rho_{AB}^*(\sigma_A^y \otimes \sigma_B^y)^\dagger$, with ρ_{AB}^* being the conjugate of ρ_{AB} in any basis, and σ_α^y is the y component of the spin-1/2 Pauli operator for the partition α $(\alpha = A,B)$. We note that all the aforementioned correlation quantifiers are measured in bits, as usual.

III. THERMAL CORRELATIONS IN THE ANISOTROPIC *XY* SPIN CHAIN

The one-dimensional XY model in a transverse field describes a chain of spins anisotropically interacting in the xy spin plane under the effect of a magnetic field in the z direction. The system is governed by the Hamiltonian

$$H = -\sum_{j=0}^{N-1}\left\{\frac{\lambda}{2}[(1+\gamma)\sigma_j^x\sigma_{j+1}^x + (1-\gamma)\sigma_j^y\sigma_{j+1}^y] + \sigma_j^z\right\}, \tag{6}$$

where σ_j^k $(k = x,y,z)$ is the k component of the spin-1/2 Pauli operator acting on site j state space, γ is the degree of anisotropy (where we take for simplicity $0 \leqslant \gamma \leqslant 1$), and λ provides the strength of the inverse of the external transverse magnetic field. We will be interested in the limit of an infinite chain, namely, $N \to \infty$.

The XY model is exactly solvable [28,29]. The Hamiltonian can be diagonalized via a Jordan-Wigner map followed by a Bogoliubov transformation (see, e.g., Ref. [30]). By taking the thermal ground state, the reduced density operator for the sites 0 and n reads [31]

$$\rho_{0n} = \frac{1}{4}\left\{I_{0n} + \langle\sigma^z\rangle(\sigma_0^z + \sigma_n^z) + \sum_{k=1}^{3}\langle\sigma_0^k\sigma_n^k\rangle\sigma_0^k\sigma_n^k\right\}, \tag{7}$$

with I_{0n} being the identity operator acting on the state space of the sites $0n$. Although an unbroken state, ρ_{0n} is able to provide an exact description of the critical behavior as well as its scaling in finite systems [31–35]. (For a detailed treatment of the spontaneous symmetry breaking at zero temperature see Refs. [36–38].)

Since the system is invariant by translations, the elements of the two-site reduced-density operator depends only on the distance (n) between the sites. The transverse magnetization is given by [28]

$$\langle\sigma^z\rangle = -\int_0^\pi \frac{(1 + \lambda\cos\phi)\tanh(\beta\omega_\phi)}{2\pi\omega_\phi}d\phi, \tag{8}$$

where $\omega_\phi = \sqrt{(\gamma\lambda\sin\phi)^2 + (1+\lambda\cos\phi)^2}/2$ and $\beta = 1/kT$ with k being Boltzmann's constant and T the absolute temperature. The two-point correlation functions read [29]

$$\langle\sigma_0^x\sigma_n^x\rangle = \begin{vmatrix} G_{-1} & G_{-2} & \cdots & G_{-n} \\ G_0 & G_{-1} & \cdots & G_{-n+1} \\ \vdots & \vdots & \ddots & \vdots \\ G_{n-2} & G_{n-3} & \cdots & G_{-1} \end{vmatrix}, \tag{9}$$

$$\langle\sigma_0^y\sigma_n^y\rangle = \begin{vmatrix} G_1 & G_0 & \cdots & G_{-n+2} \\ G_2 & G_1 & \cdots & G_{-n+3} \\ \vdots & \vdots & \ddots & \vdots \\ G_n & G_{n-1} & \cdots & G_1 \end{vmatrix}, \tag{10}$$

and

$$\langle\sigma_0^z\sigma_n^z\rangle = \langle\sigma^z\rangle^2 - G_nG_{-n}, \tag{11}$$

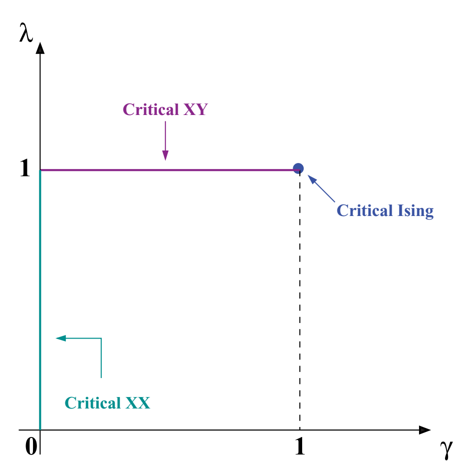

FIG. 1. (Color online) Quantum phase diagram for the anisotropic XY spin-1/2 chain. The XX model obtained by setting $\gamma = 0$ displays a critical line for $\lambda \in [0,1]$. The Ising model obtained for $\gamma = 1$ exhibits a critical point at $\lambda = 1$.

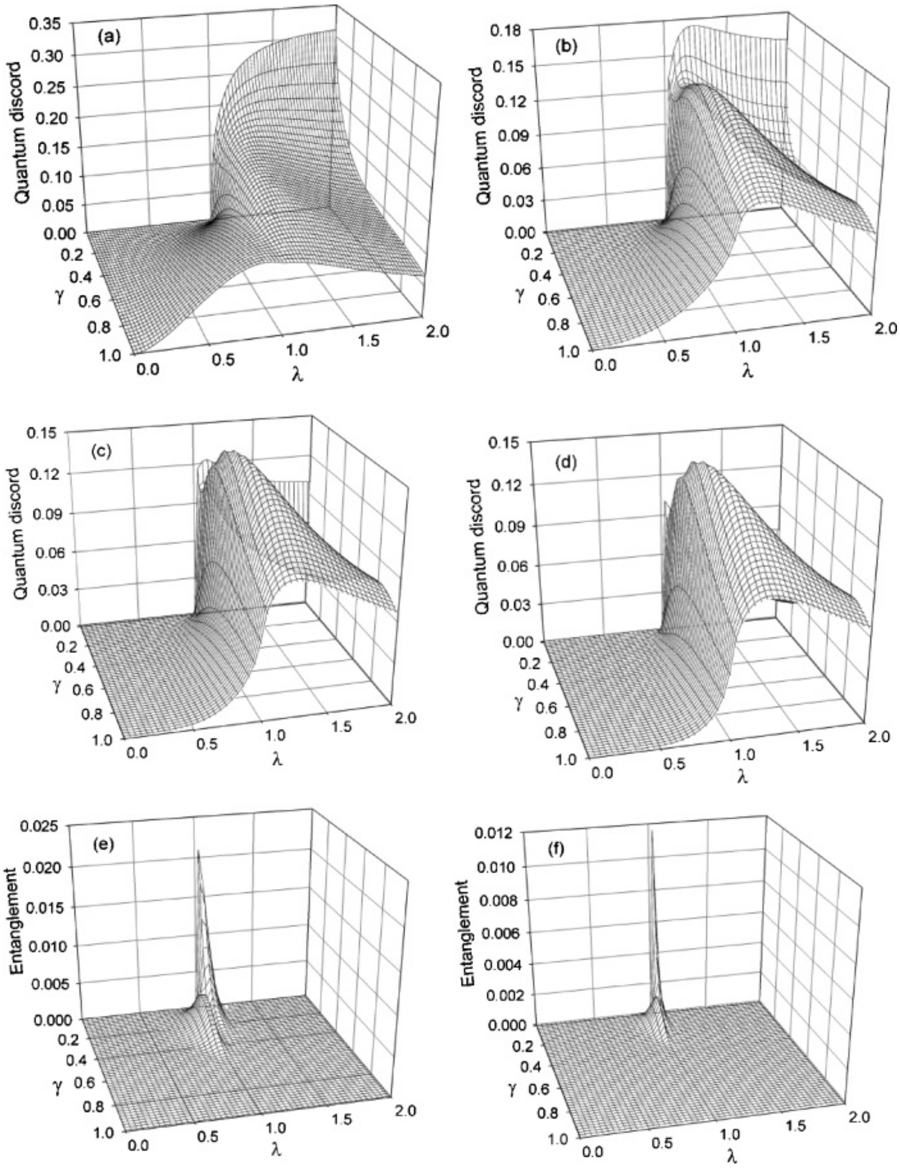

FIG. 2. Quantum discord between (a) first, (b) second, (c) third, and (d) fourth nearest neighbors and entanglement of formation between (e) third and (f) fourth nearest neighbors as a function of anisotropy (γ) and λ at zero temperature.

where

$$G_n = \int_0^{\pi} \frac{\tanh(\beta\omega_\phi)}{2\pi\omega_\phi}\{\cos(n\phi)(1+\lambda\cos\phi) - \gamma\lambda\sin(n\phi)\sin\phi\}\,d\phi. \tag{12}$$

The total correlation in (7) is quantified by the quantum mutual information as $I(\rho_{0n}) = S(\rho_0) + S(\rho_n) - S(\rho_{0n})$ with $S(\rho_0) = S(\rho_n) = -\sum_{i=0}^{1}\{[1+(-1)^i\langle\sigma^z\rangle]/2\}\log_2\{[1+(-1)^i\langle\sigma^z\rangle]/2\}$ and $S(\rho_{0n}) = -\sum_{i,j=0}^{1}(\xi_i\log_2\xi_i + \xi_j\log_2\xi_j)$, where $\xi_i = [1+\langle\sigma_0^z\sigma_n^z\rangle + (-1)^i\sqrt{(\langle\sigma_0^x\sigma_n^x\rangle - \langle\sigma_0^y\sigma_n^y\rangle)^2 + 4\langle\sigma^z\rangle^2}]/4$ and $\xi_j = [1-\langle\sigma_0^z\sigma_n^z\rangle + (-1)^j(\langle\sigma_0^x\sigma_n^x\rangle + \langle\sigma_0^y\sigma_n^y\rangle)]/4$. We can compute the QD and its classical counterpart by extremizing Eqs. (2) and (3) over the following complete set of orthonormal projectors $\{\Pi_\beta = |\Theta_\beta\rangle\langle\Theta_\beta|, \beta = \parallel, \perp\}$ onto the nth nearest neighbor, where $|\Theta_\parallel\rangle \equiv \cos(\theta/2)|0\rangle_n + e^{i\varphi}\sin(\theta/2)|1\rangle_n$ and $|\Theta_\perp\rangle \equiv e^{-i\varphi}\sin(\theta/2)|0\rangle_n - \cos(\theta/2)|1\rangle_n$. Remarkably, a numerical analysis implies that the extremization is achieved, for any values of γ, λ, and T, by the choice

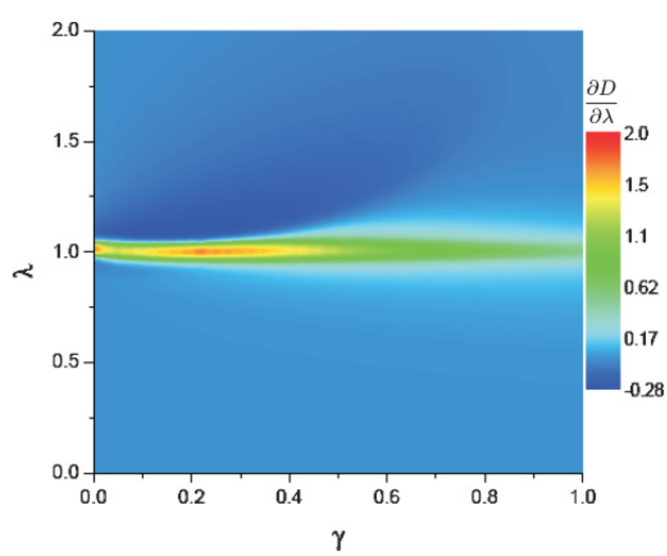

FIG. 3. (Color online) Derivative of the quantum discord between fourth nearest neighbors with respect to λ at zero temperature.

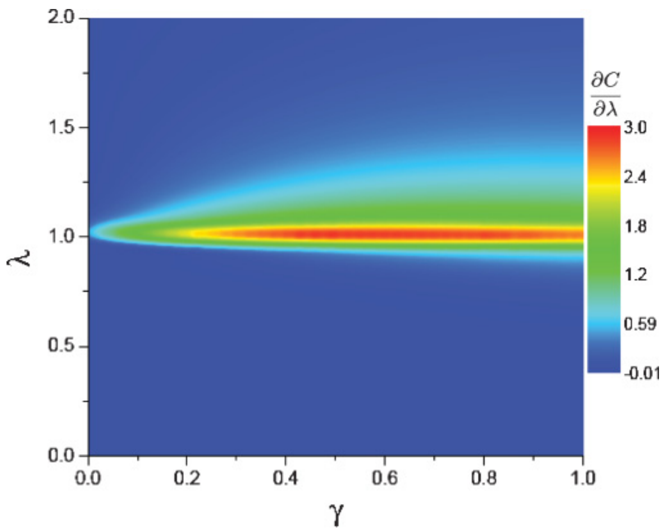

FIG. 4. (Color online) Derivative of the classical correlation between fourth nearest neighbors with respect to λ at zero temperature.

$\theta = \pi/2$ and $\varphi = 0$. Then, the relevant measurement for the model is given by $\{|+\rangle\langle+|, |-\rangle\langle-|\}$, with $|+\rangle$ and $|-\rangle$ denoting the up and down spins in the x direction, namely, $|\pm\rangle = (|\uparrow\rangle^z \pm |\downarrow\rangle^z)/\sqrt{2}$. This result generalizes the extremization obtained for the transverse field Ising model at zero temperature in Ref. [12], and it allows us to write the classical correlation as

$$C(\rho_{0n}) = \mathcal{H}_{\text{bin}}(p_1) - \mathcal{H}_{\text{bin}}(p_2), \tag{13}$$

where

$$p_1 = \frac{1}{2}(1 + \langle\sigma^z\rangle), \tag{14a}$$

$$p_2 = \frac{1}{2}\left(1 + \sqrt{\langle\sigma_0^x\sigma_n^x\rangle^2 + \langle\sigma^z\rangle^2}\right). \tag{14b}$$

Thus the quantum correlation in state (7) is simply given by

$$D(\rho_{0n}) = I(\rho_{0n}) - C(\rho_{0n}). \tag{15}$$

A. Correlations at zero temperature and QPTs

Let us first consider the XY model at zero temperature. Such a model has a quantum phase diagram displayed in Fig. 1 (see, e.g., [28,29,39]).

The QD for the first, second, third, and fourth nearest neighbors in the thermal ground state (7), close to zero temperature, is displayed in Figs. 2(a)–2(d). As expected, QD decreases as we increase the distance between the sites. However, we also see a clear difference in the amount of quantum correlation between the regions where $\lambda < 1$ and $\lambda > 1$. Although the maximum value of QD decreases as we increase the distance between the sites, the slope in the critical region gets more evident for far neighbors. The maximum increasing rate of the QD as a function of λ occurs at the quantum phase transition line ($\lambda = 1$). We also note that the nonclassical correlation is created when the magnetic field increases. The derivative of the quantum discord between fourth nearest neighbors with respect to λ is depicted in Fig. 3. So, the quantum discord between far neighbors can be used to characterize the QPT. It is important to mention that, even when entanglement is not present, the QPT can be clearly revealed through the singular behavior of QD. In Figs. 2(e) and 2(f) we note that, for a considerable range of γ, the entanglement of formation is zero (i.e., there is no entanglement) for third and fourth nearest neighbors. In the particular case of the transverse field Ising model ($\gamma = 1$), entanglement is indeed completely absent for sites farther than second nearest neighbors [32]. On the other hand, QD is non-null (where the entanglement is zero) and its behavior reveals that, for $\gamma = 1$ and $\lambda > 1$, we have a considerable amount of nonclassical correlation between far sites. It is worthwhile to observe that the pairwise classical correlation can also be employed to detect a QPT in a very evident way. In the Ising model, for example, the first derivative of the classical correlation with respect to λ is not analytic at the critical point, while the second derivative of quantum discord presents such a nonanalicity [12]. This behavior of the classical correlation also holds in the XY model for the whole range of values of γ considered here, as depicted in Fig. 4.

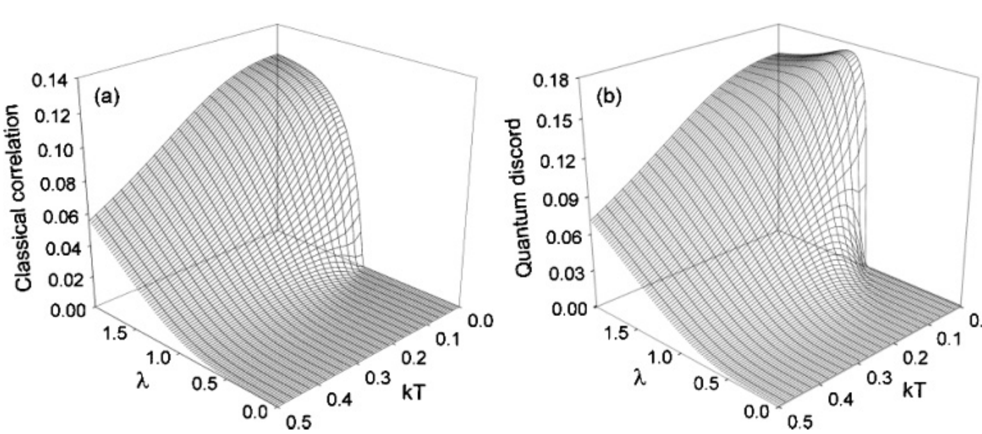

FIG. 5. (a) Classical and (b) quantum correlations between second nearest neighbors in the XX model as a function of temperature (kT) and inverse of the magnetic field (λ).

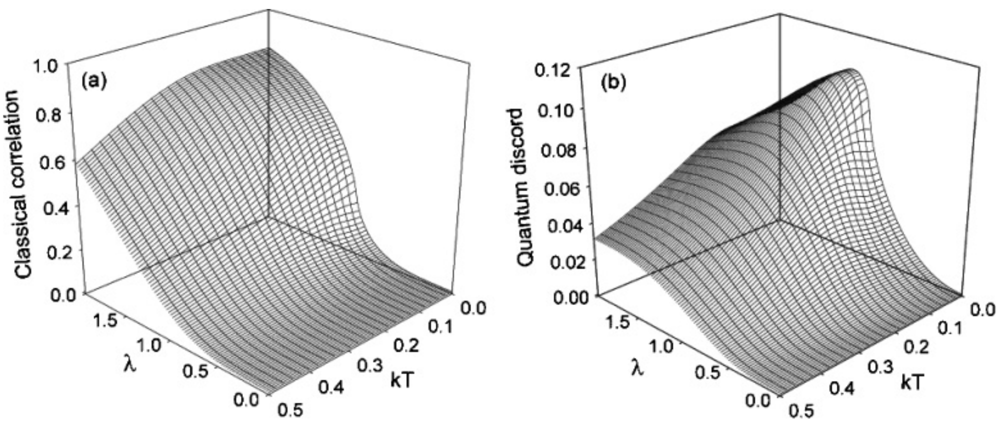

FIG. 6. (a) Classical and (b) quantum correlations between second nearest neighbors in the transverse Ising model as a function of temperature (kT) and inverse of the magnetic field (λ).

B. Correlations at finite temperatures

In order to introduce finite temperature, we begin by considering the thermal state of the XX model ($\gamma = 0$). For this limit, we plot the thermal classical and quantum correlations for the second nearest neighbors in Fig. 5. Similar results are obtained for other nearest neighbors. We note that the quantum discord is typically greater than its classical counterpart and it indeed may increases with temperature (in a given region) for some values of λ, as is evident near the critical value $\lambda = 1$. This result extends, to the thermodynamic limit, the previous analysis for two-spin Hamiltonians reported in Ref. [13]. The increase of QD with temperature when a magnetic field is present is a consequence of the fact that, when the field is turned on, the ground state tends to be less correlated than some low-lying excited states. So the effect of the temperature is to populate such correlated excited states, leading to the net effect of increasing QD. Naturally, this effect tends to disappear as the temperature gets too large. This is similar to the behavior of entanglement observed in Ref. [40].

Let us now turn our attention to the transverse Ising model ($\gamma = 1$) at finite temperatures. Classical correlation and QD for second nearest neighbors are shown in Fig. 6. Note that QD still increases with temperature but this effect is feeble when compared with the same behavior in the XX model. We also observe that the classical correlation is typically greater than the quantum discord for any temperature. This is the opposite scenario in comparison with the XX model. Remarkably, for a weak magnetic field, QD available in the XX model overcomes that of the transverse Ising model. So, applications of the XY model in QIS tends to offer more quantum correlation as a resource in the isotropic limit (the XX model) than in the Ising limit.

IV. CONCLUSION

In summary, we have examined pairwise QD and its classical counterpart in the thermodynamic limit of the anisotropic XY spin-1/2 chain in the presence of an external transverse magnetic field. We have considered the system at both zero and finite temperatures, providing an analytical expression for both classical and quantum correlations for spin pairs at any distance. Remarkably, we have shown that the quantum discord between far neighbors is able to characterize a QPT, even for distances where pairwise entanglement is absent. This is a consequence of the longer range of nonclassical correlation (that is nonvanishing for far neighbors) in comparison with the usual short-range behavior of pairwise entanglement. Concerning the thermal effect on correlations, we have shown how QD can be increased with temperature as the transverse magnetic field is varied. Moreover, we have also outlined the dominance of the QD over the classical correlation for the XX model in opposition to the Ising limit. Generalization of these results for larger subsystems and further analysis of the typical behavior of QD for quantum critical phenomena including spontaneous symmetry breaking (at zero temperature) are left for a future investigation.

Note added. Recently, we became aware of an analytical expression (see Ref. [41]) for the classical correlation in a class of states that includes the Z_2 symmetric states. Such an analytical formula confirms our numerical verification that results in Eq. (13).

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