Quantum discord in finite XY chains

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We examine the quantum discord between two spins in the exact ground state of finite spin-1/2 arrays with anisotropic XY couplings in a transverse field B. It is shown that in the vicinity of the factorizing field B_s, the discord approaches a common finite non-negligible limit which is independent of the pair separation and the coupling range. An analytic expression of this limit is provided. The discord of a mixture of aligned pairs in two different directions, crucial for the previous results, is analyzed in detail, including the evaluation of coherence effects, relevant in small samples and responsible for a parity splitting at B_s. Exact results for finite chains with first-neighbor and full-range couplings and their interpretation in terms of such mixtures are provided.

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I. INTRODUCTION

The great interest in quantum entanglement in recent years was triggered by the key role it played in certain quantum-processing tasks like quantum teleportation and superdense coding [1–3]. It was also shown to be essential for achieving an exponential speedup over classical computation in pure-state-based quantum computation [4]. However, it was recently recognized that in the case of mixed-state-based quantum computation, like the "deterministic quantum computation with one qubit" model introduced by Knill and Laflamme [5], an exponential speedup can take place without a substantial presence of entanglement [6]. This has turned attention to alternative measures of quantum correlations in mixed states, like the quantum discord introduced by Ollivier and Zurek [7], which can detect those quantum correlations present in certain separable mixed states [8] and hence not captured by the entanglement of formation [9], but which are still useful and crucial for certain quantum tasks. It was in fact recently shown by Datta, Shaji, and Caves [10] that the circuit of Ref. [5] does exhibit a finite non-negligible value of the quantum discord between the control qubit and the remaining mixed qubits. Since then, interest in quantum discord and other alternative measures has grown considerably [11–15] and several studies of their behavior in spin pairs immersed in a spin chain have been performed [16–19].

The aim of this work is to analyze the quantum discord of spin pairs in the exact ground state of *finite* spin-1/2 arrays with anisotropic XY- or XYZ-type couplings in a uniform transverse magnetic field B. The exact ground state of a finite chain has a definite spin-parity and this property is seen to deeply affect the discord for fields lower than the critical field B_c, where we show that the main results can be interpreted in terms of the discord of mixtures of aligned pairs. Our interest in these systems is motivated in particular by the remarkable factorization phenomenon they can exhibit at a particular finite value $B_s < B_c$ of the magnetic field [20–27]: At such a field, they have an exactly *separable* (i.e., factorized) ground state. This feature was first discovered in Ref. [20] in one-dimensional (1D) XY chains with first-neighbor couplings, and later shown to occur also in more general systems, like 2D arrays [22], cyclic [24] and general [25,26] arrays with arbitrary range couplings with a common anisotropy, and also systems in nonuniform fields [26]. For transverse fields, these separable ground states actually break parity symmetry and are hence degenerate, with B_s coinciding in a finite system with the last crossing of the two lowest opposite parity levels [24]. A most remarkable related feature is that, in the immediate vicinity of B_s, pairwise entanglement, although weak, reaches full range [23,24], regardless of the coupling range [24], changing at B_s from antiparallel ($B < B_s$) to parallel ($B > B_s$) type [23], indicating an "entanglement transition." This suggests the possibility of a nonzero discord between distant pairs, at least in the vicinity of B_s, with universal features (independence of separation and coupling range). Here we show that this is indeed the case, and we also derive its analytic limits at this field.

Moreover, distributed pairwise entanglement is necessarily weak due to the well-known monogamy property [28,29] associated with entanglement sharing: If in a system of n spins or qubits one spin is strongly entangled with a second spin, it cannot be strongly entangled with any of the remaining spins. This fundamental feature follows from the bound [28,29] $\sum_{j\neq i} C_{ij}^2 \leqslant C_i^2 \leqslant 1$ satisfied by the pairwise concurrences [30] C_{ij} measuring the entanglement between spins i and j, where C_i represents the concurrence between i and the rest of the chain. If all pairs are equally entangled, the maximum value that can be reached by C_{ij} is in fact just $2/n$ [31,32]. In contrast, the quantum discord is not affected by such a bound and can simultaneously reach non-negligible finite values between any two spins, as is seen to occur in the vicinity of B_s, leading to a quite different behavior with the applied field and separation in the whole region $|B| < B_c$. The properties of the ground-state discord in the vicinity of the separability field in anisotropic XY chains were not discussed in previous references. We also analyze here finite size effects, which lead to a finite step of the discord at the factorizing field B_s and other parity transitions, visible in small chains.

Section II discusses the quantum discord and its evaluation in typical reduced states of a spin pair in such chains, describing in detail the case of a mixture of two aligned states, which represents the exact reduced state in the vicinity of B_s. Coherence effects in these mixtures, relevant for small chains, are also examined. Section III discusses the behavior of the discord of spin pairs with the applied field and separation in finite cyclic XY chains with first-neighbor as well as full-range couplings, including its interpretation and the differences with the pair entanglement. The Appendix discusses the details of the exact definite parity solution of the finite cyclic XY chain. Conclusions are finally drawn in Sec. IV.

II. FORMALISM

A. Quantum discord

The quantum discord (D) is a measure of quantum correlations based on the difference between two distinct quantum generalizations of the classical mutual information, or equivalently, the classical conditional entropy [7,10]. Given a bipartite system $A+B$ in a mixed state ρ_{AB}, and denoting with $\rho_A = \mathrm{Tr}_B\rho_{AB}$, $\rho_B = \mathrm{Tr}_A\rho_{AB}$ the reduced density operators of each subsystem, D can be expressed as [7]

$$D = I(A:B) - \max_{\{P_j^B\}} I_{\{P_j^B\}}(A:B) \tag{1a}$$

$$= \min_{\{P_j^B\}}[S(\rho'_{AB}) - S(\rho'_B)] - [S(\rho_{AB}) - S(\rho_B)], \tag{1b}$$

where $I(A:B) = S(\rho_A) + S(\rho_B) - S(\rho_{AB}) \geqslant 0$ is the quantum mutual information, with $S(\rho) = -\mathrm{Tr}\rho\log_2\rho$ the von Neumann entropy, and $I_{\{P_j^B\}}(A:B) = S(\rho_A) + S(\rho'_B) - S(\rho'_{AB})$ the mutual information after a local von Neumann measurement in system B defined by a set of orthogonal projectors $P_j^B = I_A \otimes |j_B\rangle\langle j_B|$. Here

$$\rho'_{AB} = \sum_j P_j^B \rho_{AB} P_j^B \tag{2}$$

represents the joint state after such measurement if the result is unknown, with $\rho'_B = \mathrm{Tr}_A\rho'_{AB}$ and $\rho'_A = \mathrm{Tr}_B\rho'_{AB} = \rho_A$. Minimization in (1b) is over all sets of local projectors.

The last bracket in (1b) is the direct quantum extension of the classical conditional entropy [3,33] [$S(A|B) = S(A,B) - S(B) = \sum_j p_j S(A/j)$, with $S(A,B) = -\sum_{i,j} p_{ij}\log_2 p_{ij}$, $S(B) = -\sum_j p_j^B \log_2 p_j^B$, and $S(A/j) = -\sum_j (p_{ij}/p_j^B)\log_2(p_{ij}/p_j^B)$ for a system with joint probability distribution p_{ij} and marginal distribution $p_j^B = \sum_i p_{ij}$], which, in contrast with the classical case, is not necessarily positive. On the other hand, the first bracket is the conditional entropy $S_{\{P_j^B\}}(A|B) = \sum_j p_j S(\rho_j)$ after a local measurement in system B, where $p_j = \mathrm{Tr}P_j^B\rho_{AB}$ is the probability of outcome j and $\rho_j = P_j^B\rho_{AB}P_j^B/p_j$ the state after such an outcome. It represents the average lack of information about A after such measurement and is a nonnegative quantity. The second term in (1a) is considered a measure of the *classical* correlations between A and B in Ref. [34], the discord then measuring the quantum part of these correlations.

In the case of a pure state ($\rho_{AB}^2 = \rho_{AB}$), $S(\rho_{AB}) = 0$ while the first bracket in (1b) vanishes for any choice of local projectors, and the discord then reduces to the entanglement entropy [35] $D = E = S(\rho_A) = S(\rho_B)$. In the case of mixed states, however, it does not coincide in general with the entanglement of formation [9] (the convex roof extension of the entanglement entropy). While the latter vanishes for any separable state (i.e., for a convex superposition of product states $\rho_{AB} = \sum_\alpha q_\alpha \rho_A^\alpha \otimes \rho_B^\alpha$, $q_\alpha \geqslant 0$ [8]), the discord can be nonzero for these states. The discord vanishes in the case of densities diagonal in an orthogonal product basis ($b_{AB} = \{|i_A\rangle|j_B\rangle\}$) or in general a conditional product basis ($b_{AB} = \{|i_{jA}\rangle|j_B\rangle\}$, with the orthogonal set $\{|i_{jA}\rangle\}$ depending on $|j_B\rangle$), but it does not vanish in general for a mixture of noncommuting product states, which is still a separable state. The difference (1) can be shown to be non-negative [7] due to the subtle concavity property of the *conditional* von Neumann entropy $S(\rho_{AB}) - S(\rho_B)$ [33].

B. Quantum discord and entanglement of spin pairs in definite parity states

Let us now describe the basic elements to evaluate the discord and entanglement of a spin pair in a typical eigenstate of a finite chain of n spins, where the rest of the spins play the role of an environment. We consider spin-1/2 chains with XYZ couplings of arbitrary range in a uniform transverse magnetic field B along the z axis, such that the chain Hamiltonian has the form

$$H = B\sum_i s_{iz} - \frac{1}{2}\sum_{i\neq j}\sum_{\mu=x,y,z} J_\mu^{ij} s_{i\mu}s_{j\mu}, \tag{3}$$

where $s_{i\mu}$ denotes the spin components at site i (in units of $\hbar$). H commutes with the spin-parity operator

$$P_z = \exp\left[i\pi\sum_i(s_{iz}+1/2)\right] = \prod_i(-\sigma_{iz}), \tag{4}$$

where $\sigma_{iz} = 2s_{iz}$, which changes $s_{i\mu}$ to $-s_{i\mu}$ $\forall i$ and $\mu = x,y$. Nondegenerate eigenstates $|\Psi_\nu\rangle$ of H then have a definite spin-parity $P_z = \pm 1$, a symmetry which plays a fundamental role in our discussion.

The reduced density matrix of an arbitrary pair i,j in such an eigenstate,

$$\rho_{ij} = \mathrm{Tr}_{n-ij}|\Psi_\nu\rangle\langle\Psi_\nu|, \tag{5}$$

then contains no elements connecting states of opposite parity, commuting therefore with the pair parity $P_z^{ij} = \sigma_{iz}\sigma_{jz}$. In the standard basis $\{|00\rangle,|01\rangle,|10\rangle,|11\rangle\}$ ($|kl\rangle \equiv |k_i\rangle|l_j\rangle$, with $s_{iz}|k_i\rangle = \frac{1}{2}e^{i\pi k_i}|k_i\rangle$, $k_i = 0,1$), ρ_{ij} is then of the form

$$\rho_{ij} = \begin{pmatrix} a & 0 & 0 & \alpha \\ 0 & c & \beta & 0 \\ 0 & \bar\beta & c' & 0 \\ \bar\alpha & 0 & 0 & b \end{pmatrix}, \tag{6}$$

where, setting $\langle O\rangle \equiv \mathrm{tr}\rho_{ij}O$ and $s_{i\pm} = s_{ix} \pm i s_{iy}$,

$$\begin{pmatrix} a \\ b \end{pmatrix} = \frac{1}{4} \pm \frac{1}{2}\langle s_{iz}+s_{jz}\rangle + \langle s_{iz}s_{jz}\rangle, \tag{7}$$

$$\begin{pmatrix} c \\ c' \end{pmatrix} = \frac{1}{4} \pm \frac{1}{2}\langle s_{iz}-s_{jz}\rangle - \langle s_{iz}s_{jz}\rangle, \tag{8}$$

$$\begin{pmatrix}\alpha\\ \beta\end{pmatrix} = \langle s_{i-}s_{j\mp}\rangle, \tag{9}$$

with $a+b+c+c'=1$. Here we consider translationally invariant systems such that $\langle s_{iz}\rangle = \langle s_{jz}\rangle$ and hence $c=c'=\frac{1}{2}(1-a-b)$. Moreover, α and β are real since H can be represented by a real matrix in the standard product basis of the full space. Non-negativity of ρ_{ij} implies $|\alpha| \leqslant \sqrt{ab}$, $|\beta| \leqslant c$, with a, b, and c non-negative.

The internal entanglement of the pair can be measured through the entanglement of formation, which for the case of two qubits can be explicitly calculated as [30]

$$E = -\sum_{\nu=\pm} q_\nu \log_2 q_\nu, \quad q_\pm = \frac{1}{2}(1 \pm \sqrt{1-C^2}), \tag{10}$$

where C is the *concurrence* [30]. It is given here by

$$C = 2\max[|\alpha| - c, |\beta| - \sqrt{ab}, 0]. \tag{11}$$

The entanglement of the pair is of parallel (antiparallel) type if the first (second) entry is positive [23,24]. Just one of these entries can be positive for a non-negative ρ_{ij}. On the other hand, in order to evaluate the discord of the pair, we first need the eigenvalues of ρ_{ij}, given for $c=c'$ by $\lambda_{ij} = (\frac{1-a-b}{2} \pm |\beta|, \frac{a+b}{2} \pm \sqrt{(\frac{a-b}{2})^2 + |\alpha|^2})$, and those of the single spin-density matrix,

$$\rho_j = \mathrm{Tr}_i\,\rho_{ij} = \begin{pmatrix} a+c & 0\\ 0 & c+b\end{pmatrix}, \tag{12}$$

which are obviously $\lambda_j = \frac{1}{2}[1 \pm (a-b)]$. We also need to consider a measurement of the spin at site j along an arbitrary axis z' defined by the angles γ and ϕ. The state of the pair after such measurement [Eq. (2)] is

$$\rho'_{ij} = P^j_{0'}\rho_{ij}P^j_{0'} + P^j_{1'}\rho_{ij}P^j_{1'}, \tag{13}$$

where $P^j_{k'} = I_i \otimes |k'\rangle\langle k'|$ for $k=0,1$ with

$$|0'\rangle = \cos\left(\tfrac{1}{2}\gamma\right)|0\rangle + e^{i\phi}\sin\left(\tfrac{1}{2}\gamma\right)|1\rangle \tag{14}$$

$$|1'\rangle = \cos\left(\tfrac{1}{2}\gamma\right)|1\rangle - e^{-i\phi}\sin\left(\tfrac{1}{2}\gamma\right)|0\rangle, \tag{15}$$

such that $s_{jz'}|k'\rangle = \frac{1}{2}e^{i\pi k}|k'\rangle$ for $s_{jz'} = s_{jz}\cos\gamma + s_{jx}\sin\gamma\cos\phi + s_{jy}\sin\gamma\sin\phi$. For real α,β, the eigenvalues of ρ'_{ij} are

$$\lambda'_{ij} = \frac{1 + \nu(a-b)\cos\gamma + \mu\sqrt{[(2(a+b)-1)\cos\gamma + \nu(a-b)]^2 + 4(\alpha^2+\beta^2+2\alpha\beta\cos2\phi)\sin^2\gamma}}{4}, \tag{16}$$

where $\nu = \pm1$, $\mu = \pm1$, corresponding $\nu = 1$ (-1) to the eigenvalues of the first (second) term in Eq. (13). The eigenvalues of $\rho'_j = \mathrm{Tr}_i\,\rho'_{ij}$ are then $\lambda'_j = \frac{1}{2}[1 \pm (a-b)\cos\gamma]$.

We then have all elements to evaluate the difference

$$D(\gamma,\phi) = S(\rho'_{ij}) - S(\rho'_j) - [S(\rho_{ij}) - S(\rho_j)], \tag{17}$$

whose minimum (with respect to θ,ϕ) is the discord D [Eq. (1)]. For $\alpha\beta \geqslant 0$, minimization with respect to ϕ yields $\cos 2\phi = 1$ and just the minimization over γ is finally required, which can be restricted to the interval $[0,\pi/2]$. The minimum for the pair densities used in Sec. III was obtained for $\gamma = \pi/2$ $(z'=x)$, where $\lambda'_{ij} = \frac{1+\mu\sqrt{(a-b)^2+4(\alpha+\beta)^2}}{4}$ becomes independent of ν and hence degenerate. A general evaluation of the discord for states of the form (6) was recently provided [14].

C. The case of a mixture of two aligned states

A particular case of Eq. (6) of exceptional interest is that of a statistical mixture of two aligned states along arbitrary directions, not necessarily opposite, such that the local states involved are *nonorthogonal*. Choosing the z axis as the bisector of the angle between the two directions, we can write this state as

$$\rho_{ij}(\theta) = \tfrac{1}{2}(|\theta\theta\rangle\langle\theta\theta| + |-\theta-\theta\rangle\langle-\theta-\theta|) \tag{18}$$

$$= \begin{pmatrix} a & 0 & 0 & \alpha\\ 0 & \alpha & \alpha & 0\\ 0 & \alpha & \alpha & 0\\ \alpha & 0 & 0 & b\end{pmatrix}, \quad \begin{matrix}\binom{a}{b} = \frac{1}{4}(1\pm\cos\theta)^2\\ \alpha = \frac{1}{4}\sin^2\theta\end{matrix}, \tag{19}$$

where $|\theta\rangle = \exp[-i\theta s_{iy}]|0\rangle = \cos\frac{1}{2}\theta|0\rangle + \sin\frac{1}{2}\theta|1\rangle$ and Eq. (19) is again the standard basis representation. Equation (18) is the exact reduced state of any two spins in the immediate vicinity of the factorizing field (see Sec. III) if coherence terms are neglected. It also provides the basic approximate picture of the pair state in the region $|B| < B_c$.

The state (18) is obviously separable [8] (i.e., a convex combination of product states), and therefore its concurrence and entanglement are identically zero, as verified from Eq. (11). However, its discord is positive for $\theta \in (0,\pi/2)$, vanishing just for $\theta = 0$ or $\theta = \pi/2$: If $\theta = 0$, Eq. (18) becomes a pure product state [and hence $D(\gamma,\phi) = 0\ \forall\ \gamma,\phi$], whereas if $\theta = \pi/2$, $|\theta\rangle$ and $|-\theta\rangle$ are orthogonal and $\rho(\theta)$ becomes diagonal in a product basis, with Eq. (17) vanishing then for $\gamma = \pi/2$ and $\phi = 0$ $(\rho'_{ij} = \rho_{ij})$.

In the general case, the eigenvalues of Eq. (19) are $\lambda_{ij} = (\frac{1}{2}(1 \pm \cos^2\theta), 0, 0)$, with those of $\rho_j(\theta)$ given by $\lambda_j = \frac{1}{2}(1 \pm \cos\theta)$, whereas the ensuing eigenvalues (16) of ρ'_{ij} become, for $\cos 2\phi = 1$,

$$\lambda'_{ij} = \frac{1 + \nu\cos\theta\cos\gamma + \mu\sqrt{[(1+\nu\cos\theta\cos\gamma)^2\cos^2\theta + \sin^2\gamma\sin^4\theta}}{4} \tag{20}$$

with those of ρ'_j given by $\lambda'_j = \frac{1}{2}(1 \pm \cos\theta\cos\gamma)$. For $\theta \in (0,\pi/2]$, the minimum of Eq. (17) is always attained at $\gamma = \pi/2$ (and $\cos 2\phi = 1$), that is, for a local measurement along the x axis, as seen in Fig. 1, with $D(\gamma,0)$ becoming quite flat for small θ. Both $\gamma = \pi/2$ and $\gamma = 0$ are stationary points of D, with 0 a maximum. Figure 2 depicts the minimum $D \equiv D(\pi/2,0)$, which is the discord, as a function of θ, given explicitly by

$$D = \sum_{\mu=\pm1}\left\{\left[2h\left(\frac{1+\mu\sqrt{1-\frac{1}{4}\sin^2 2\theta}}{4}\right) - h\left(\frac{1}{2}\right)\right] - \left[h\left(\frac{1+\mu\cos^2\theta}{2}\right) - h\left(\frac{1+\mu\cos\theta}{2}\right)\right]\right\}, \tag{21}$$

where $h(x) = -x\log_2 x$. D is a maximum at $\theta = \theta_m \approx 1.15\pi/4$, where $D \approx 0.15$. As seen in the bottom of Fig. 2, while $S(\rho'_{ij}) - S(\rho'_j)$ [the first bracket in Eq. (21)] is an even function of $\theta - \pi/4$, $S(\rho_{ij}) - S(\rho_j)$ (the last bracket) is not, being a maximum at $\theta \approx 0.91\pi/4$ and originating the deviation of θ_m from $\pi/4$.

For $\theta \to 0$, D vanishes quadratically ($D \approx \frac{1}{2}\theta^2$) while for $\theta \to \frac{\pi}{2}$, $D \approx -\frac{1}{4}(\frac{\pi}{2}-\theta)^2[\log_2(\frac{\pi}{2}-\theta)^2 + \log_2 e - 2]$.

D. Effects of coherence term

The reduced state of two spins at the factorizing field actually contains a small coherence term $\propto \varepsilon(|\theta\theta\rangle\langle-\theta-\theta| + |-\theta-\theta\rangle\langle\theta\theta|)$ (see Sec. III), which leads to the state

$$\rho^{\varepsilon}_{ij}(\theta) = \frac{|\theta\theta\rangle\langle\theta\theta| + |-\theta-\theta\rangle\langle-\theta-\theta| + \varepsilon(|\theta\theta\rangle\langle-\theta-\theta| + \text{H.c.})}{2(1+\varepsilon\langle\theta\theta|-\theta-\theta\rangle)} \tag{22}$$

$$= \begin{pmatrix} a & 0 & 0 & \alpha \\ 0 & \beta & \beta & 0 \\ 0 & \beta & \beta & 0 \\ \alpha & 0 & 0 & b \end{pmatrix}, \quad \begin{matrix} \binom{a}{b} = \frac{(1+\varepsilon)(1\pm\cos\theta)^2}{4(1+\varepsilon\cos^2\theta)} \\ \binom{\alpha}{\beta} = \frac{(1\pm\varepsilon)\sin^2\theta}{4(1+\varepsilon\cos^2\theta)} \end{matrix}, \tag{23}$$

where $|\varepsilon| \leqslant 1$. This term then generates a parity-dependent correction to the previous results. The eigenvalues of ρ_{ij} and ρ_j are now $\lambda_{ij} = (a+b, 2\beta, 0, 0)$, $\lambda_j = (a+\beta, b+\beta)$, whereas those of ρ'_{ij} and ρ'_j can be obtained from Eq. (16). The minimum of Eq. (17) is again obtained at $\gamma = \pi/2$ (and $\phi = 0$, the surface being again similar to that of Fig. 1), leading to

$$D = \sum_{\mu=\pm1}\left\{\left[2h\left(\frac{1}{4} + \mu\frac{\sqrt{\cos^2\theta(1+\varepsilon)^2 + \sin^4\theta}}{4(1+\varepsilon\cos^2\theta)}\right) - h\left(\frac{1}{2}\right)\right] - \left[h\left(\frac{(1+\mu\cos^2\theta)(1+\mu\varepsilon)}{2(1+\varepsilon\cos^2\theta)}\right) - h\left(\frac{(1+\mu\cos\theta)(1+\mu\varepsilon\cos\theta)}{2(1+\varepsilon\cos^2\theta)}\right)\right]\right\}. \tag{24}$$

For $\varepsilon \neq 0$, a nonzero entanglement of the pair also arises, with concurrence

$$C = \frac{|\varepsilon|\sin^2\theta}{1+\varepsilon\cos^2\theta}, \tag{25}$$

which is parallel (antiparallel) for $\varepsilon > 0$ ($\varepsilon < 0$).

In the limit $\varepsilon \to \pm1$, Eq. (22) becomes a pure state, namely, $\rho_{ij} \to |\Psi_\pm\rangle\langle\Psi_\pm|$ with

$$|\Psi_\pm\rangle = \frac{|\theta\theta\rangle \pm |-\theta-\theta\rangle}{\sqrt{2(1\pm\cos^2\theta)}} = \begin{cases} \frac{\cos^2\frac{\theta}{2}|00\rangle + \sin^2\frac{\theta}{2}|11\rangle}{\sqrt{(1+\cos^2\theta)/2}} \\ \frac{|01\rangle+|10\rangle}{\sqrt{2}} \end{cases}.$$

Therefore, D and E merge $\forall\,\theta$ in this limit. Whereas $|\Psi_-\rangle$ is a Bell state independent of θ (for $\theta \neq 0$), leading to $D = E = C = 1$, the entanglement of $|\Psi_+\rangle$ depends on θ [with $C = \sin^2\theta/(1+\cos^2\theta) \leqslant 1$], increasing with increasing $\theta \in [0,\pi/2]$.

The response of D and E to the coherence term is shown in Fig. 3. For sufficiently small ε, the correction to D is linear in ε for θ not close to $\pi/2$, with the discord increasing (decreasing) for $\varepsilon < 0$ ($\varepsilon > 0$), while at $\theta = \pi/2$ the correction is quadratic and positive [at $\theta = \pi/2$, $D = 1 - \sum_{\mu=\pm1} h(\frac{1+\mu\varepsilon}{2}) \approx \frac{1}{2}\varepsilon^2\log_2 e$]. Entanglement, on the other hand, becomes finite as soon as $|\varepsilon|$ increases, becoming even larger than the discord for θ close to $\pi/2$ (where $C = |\varepsilon|$ and $E \propto -\varepsilon^2\log\varepsilon^2$ for small ε). As seen in the bottom of Fig. 3, at an intermediate θ entanglement remains smaller than the discord just in an interval around $\varepsilon = 0$, becoming slightly

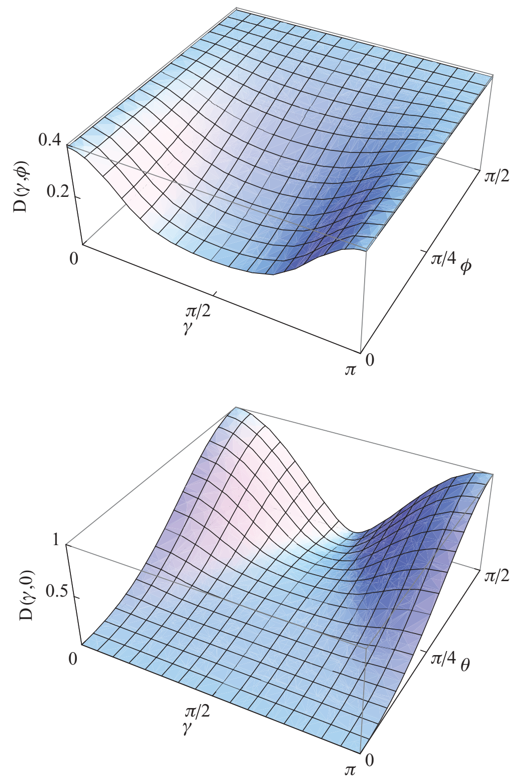

FIG. 1. (Color online) The difference (17) for the mixture (18) (top) as a function of γ and ϕ at fixed $\theta = \pi/4$ and (bottom) as a function of γ and θ at $\phi = 0$. $D(\gamma,\phi)$ is a minimum at $\gamma = \pi/2$ and $\phi = 0\ \forall\ \theta \in (0,\pi/2]$.

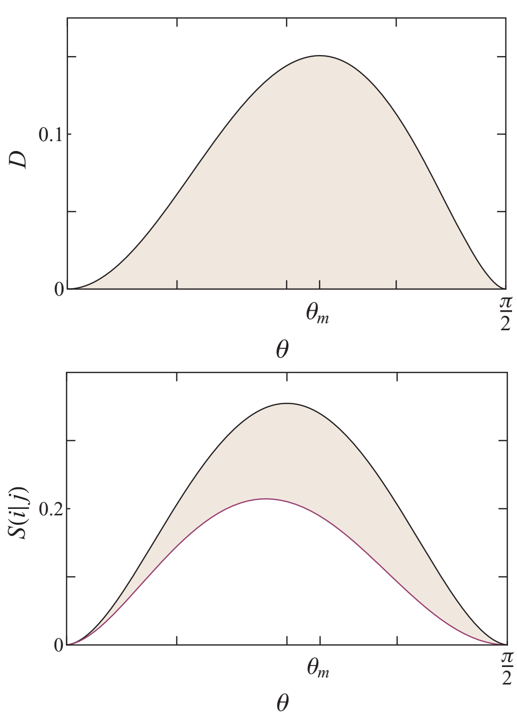

FIG. 2. (Color online) (top) Quantum discord $D \equiv D(\pi/2,0)$ as a function of θ for the state (18). D is maximum at $\theta = \theta_m \approx 1.15\pi/4$. (bottom) Conditional entropies $S(\rho'_{ij}) - S(\rho'_j)$ (upper curve) and $S(\rho_{ij}) - S(\rho_j)$ (lower curve) as a function of θ, whose difference is the discord of the top panel.

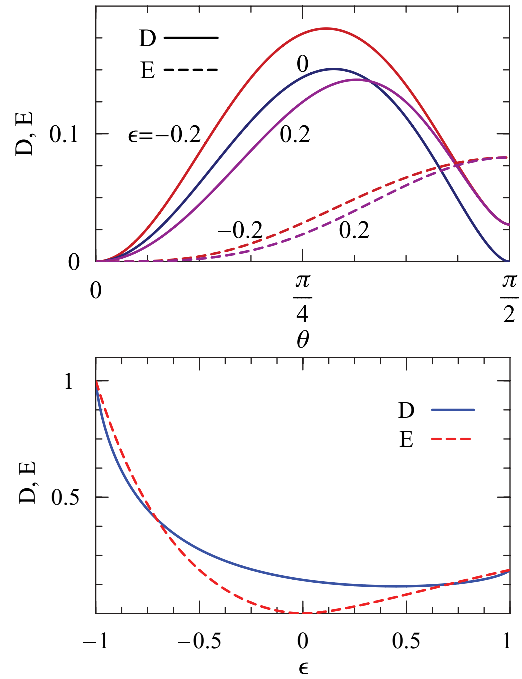

FIG. 3. (Color online) Effect of coherence term. The quantum discord (D) and entanglement of formation (E) of the state (22) (top) as a function of θ for $\varepsilon = 0.2$, 0, and -0.2 and (bottom) as a function of ε at $\theta = \pi/4$. Entanglement vanishes at $\varepsilon = 0$ but becomes larger than the discord close to the pure-state limit $\varepsilon = \pm 1$, where D and E coincide.

larger before reaching the pure limit $\varepsilon = \pm 1$, where D and E coincide.

III. QUANTUM DISCORD IN XY CHAINS

We have now all the elements to evaluate and understand the behavior of the discord of an arbitrary spin pair in the ground state of a finite chain. We first consider a finite 1D XY cyclic chain of n spins with first-neighbor couplings, where $J_z^{ij} = 0$ and

$$J_\mu^{ij} = \delta_{j,i\pm 1} J_\mu, \quad \mu = x,y, \tag{26}$$

with $n + 1 \equiv 1$. The exact solution for finite n can be obtained through the Jordan-Wigner fermionization [36] (see the Appendix). The exact ground state will have a definite (field-dependent) spin-parity and the reduced density of an arbitrary pair will be of the form (6), where the elements (7)–(9) can be evaluated with the expressions of the Appendix.

Exact results for the discord and entanglement of pairs are shown in Figs. 4 and 5 for $\chi = J_y/J_x = 0.5$ and two different values of n. For a first-neighbor coupling and even n, the sign of J_x can be changed by a local transformation $s_{2i,\mu} \to -s_{2i,\mu}$ for $\mu = x,y$, so that both the ferromagnetic ($J_x > 0$) and the antiferromagnetic ($J_x < 0$) cases at fixed χ exhibit exactly the same entanglement and discord. They are also independent of the sign of B.

It is immediately seen that pair entanglement and discord exhibit significant differences for fields $|B| < B_c = \frac{1}{2}(1+\chi)J_x$ (the critical field of the thermodynamic limit

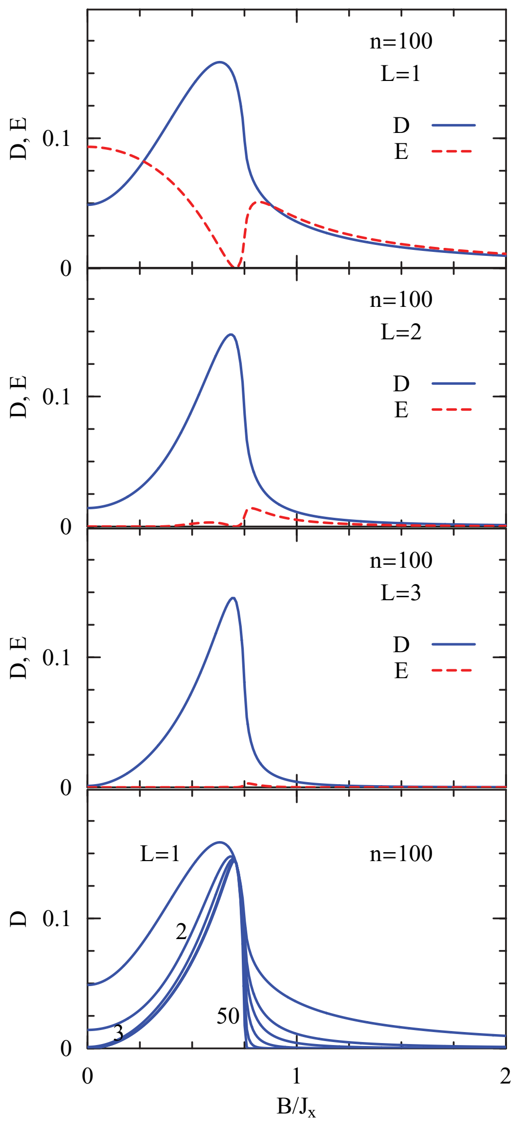

FIG. 4. (Color online) Quantum discord (D) and entanglement (E) of spin pairs with separation L in the exact ground state of a cyclic chain of $n = 100$ spins with first-neighbor XY couplings and $J_y/J_x = 0.5$, as a function of the transverse magnetic field. $L = 1$ denotes first neighbors. At the factorizing field $B_s = \sqrt{J_yJ_x} \approx 0.71J_x$, E vanishes, whereas D approaches the same finite limit (21) $\forall\, L$, with θ determined by Eq. (29). The bottom panel depicts the discord for all separations L. A finite saturation limit is approached for large L if $|B| < B_c = 0.75J_x$.

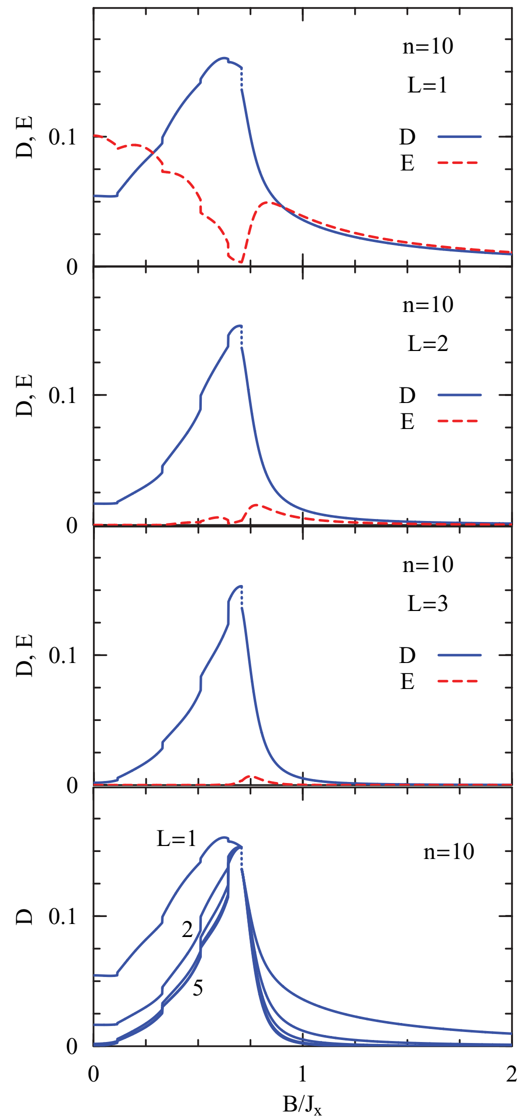

FIG. 5. (Color online) Same details as Fig. 4 for a chain with $n = 10$ spins. The common different side limits of D at the factorizing field, given by Eq. (24) with coherence factor (33), are now appreciable.

$n \to \infty$). While in this case entanglement practically vanishes at the factorizing field [20,21,23–25]

$$B_s = \sqrt{J_yJ_x}, \tag{27}$$

where the chain possesses an exactly separable and degenerate parity-breaking ground state [24] [see Eq. (28)], the discord remains nonzero, in fact reaching its maximum in its vicinity. Besides, entanglement rapidly decreases as the separation L between the spins increases, being nonzero for $L > 2$ only in the immediate vicinity of B_s, where it is very small. In contrast, the discord decreases only slightly with separation for $|B| < B_c$, reaching a saturation value for large L. Moreover, it is strictly *independent* of L at the factorizing field B_s.

In order to understand these results, we recall that at $B = B_s$ the uniform parity-breaking separable state

$$|\Theta\rangle = \otimes_{i=1}^{n}|\theta_i\rangle, \quad |\theta_i\rangle = \exp[i\theta s_{iy}|0_i\rangle, \tag{28}$$

$$\cos\theta = B_s/J_x = \sqrt{\chi}, \tag{29}$$

where here $s_{iz}|0_i\rangle = -\frac{1}{2}|0_i\rangle$, is an *exact* ground state [we have assumed $J_x > 0$; for $J_x < 0$, $\theta_i \to (-1)^i\theta$]. It is obviously a state with spins fully aligned along an axis forming an angle θ with the original $-z$ axis. Due to parity symmetry, the partner state $|-\Theta\rangle = P_z|\Theta\rangle$ is also an exact ground state at B_s. They can therefore be exact eigenstates of H only when levels of opposite parity cross [24]. The ground state of the present chain actually undergoes $n/2$ spin-parity transitions as the field B increases from 0 (reminiscent of the $m/2$ S_z transitions of the XX limit [37]), with the last one precisely at B_s. Outside these transitions, the energy gap between the lowest states of each parity is small for $|B| \lesssim B_c$, but nonetheless *finite* in a finite chain.

In the immediate vicinity of B_s, the exact ground state therefore possesses a definite parity, and the correct side limits at B_s are determined by the states

$$|\Theta^{\pm}\rangle = \frac{|\Theta\rangle \pm |-\Theta\rangle}{\sqrt{2(1 \pm \langle -\Theta|\Theta\rangle)}}, \tag{30}$$

where $\langle -\Theta|\Theta\rangle = \cos^n\theta$ [24]. The reduced state of *any* two spins derived from Eq. (30) is given precisely by the same mixture (18) (with $z \to -z$) if the complementary overlap $\langle -\Theta_{n-2}|\Theta_{n-2}\rangle = \cos^{n-2}\theta$ is neglected. We can then immediately understand the qualitative difference between entanglement and discord for $|B| < B_c$. As B approaches B_s, the discord between *any* two spins approaches a common finite limit for *any* separation L, given by Eq. (21) with θ obtained from Eq. (29) ($D \approx 0.145$ in the case of Fig. 4, where $\theta = \pi/4$ at B_s). In contrast, the pair entanglement vanishes for $B \to B_s$ (for a negligible complementary overlap) as the state (18) is separable.

In Figs. 4 and 5 we have taken the exact ground state with its correct parity. The non-negligible discord between any two spins for $|B| < B_c$ can then be understood in a similar way, because in this region the ground state can be seen, approximately, as a definite parity combination (30) of "mean-field" states with broken symmetry (28), with $\cos\theta = B/J_x$, plus additional corrections. The reduced state of a spin pair is then again given essentially by the mixture $\rho(\theta)$ [Eq. (18)] plus smaller corrections, with the discord arising principally from $\rho(\theta)$ (although corrections are non-negligible; see Fig. 6).

Let us remark that the same reduced density (18) arises from the statistical mixture $\rho_0 = \frac{1}{2}(|\Theta^+\rangle\langle\Theta^+| + |\Theta^-\rangle\langle\Theta^-|)$ if the overlap is discarded; ρ_0 represents the $T \to 0^+$ limit of the thermal state of the system at B_s. The limit (21) of the discord at B_s remains then also valid at sufficiently low T.

On the other hand, for strong fields $B \gg J_x$, the ground state is essentially the state with all spins fully aligned along the $-z$ axis plus small perturbative corrections. As seen in Fig. 4, the discord in this region is rather small and decreases rapidly with separation, since the previous superposition effects are no longer present. Moreover, the discord between first neighbors is very close to the entanglement of formation, as verified by a perturbative expansion: For $|B| \gg J_x$ and $L = 1$ in the case of Eq. (26) we obtain, setting $\eta = (J_x - J_y)/(8B)$,

$$D \approx \eta^2(-\log_2\eta^2 + \log_2 e - 2), \tag{31}$$

$$E \approx \eta^2(-\log\eta^2 + \log_2 e). \tag{32}$$

Thus, E in this region is slightly *greater* than D, as verified in the top of Figs. 4 and 5.

Results for a small chain of $n = 10$ spins are shown in Fig. 5. Although the behavior is similar to that for $n = 100$, finite size effects become important and the overlap $\langle -\Theta|\Theta\rangle$ can no longer be neglected. The effects on the discord and entanglement of the ground-state parity transitions taking place for $|B| < B_s$ are now visible, giving rise to small steps in these quantities. The final step takes place at B_s, where D now exhibits a *finite discontinuity* due to the parity splitting arising from the coherence term (Sec. II D), no longer negligible: The actual reduced state of a spin pair derived from the states (30) is given by Eq. (22) with

$$\varepsilon = \pm\cos^{n-2}\theta, \tag{33}$$

where the $-$ $(+)$ sign corresponds to the left (right) side at B_s, that is, negative (positive) spin-parity. The side limits of D at B_s are then given by Eq. (24) for the values from Eqs. (29)–(33) for θ and ε (leading to $D_- \approx 0.153$, $D_+ \approx 0.137$ in the case of Fig. 5). Small but nonzero common side limits at B_s of the entanglement between any two spins also arise [24], as determined by Eqs. (10) and (25). In contrast with the discord, Eq. (25) of course satisfies the monogamy inequality [28,29], reaching its maximum value $2/n$ in the XX limit $J_y \to J_x$ (where $\theta \to 0$ and $C(\varepsilon) \to 0$ but $C(-\varepsilon) \to 2/n$, as $|\Theta^-\rangle$ approaches the W state [24]).

The present values of the discord at the factorizing field, determined by Eqs. (21) or in general Eq. (24), are actually much more general: Uniform chains or arrays with ferromagnetic ($J_x^{ij} > 0$) XY couplings of *arbitrary* range but *common* anisotropy $\chi = J_y^{ij}/J_x^{ij} \in (0,1)$ also exhibit a factorizing field, given for spin 1/2 by [24,25]

$$B_s = \sqrt{\chi}\sum_{j\neq i} J_x^{ij}, \tag{34}$$

where the chain again possesses the same degenerate separable ground states (28). Side limits at B_s are then determined by the same definite parity states (30). The same occurs in XYZ arrays if $\chi = (J_y^{ij} - J_z^{ij})/(J_x^{ij} - J_z^{ij})$ is constant and $\in (0,1)$ [24], with $B_s = \sqrt{\chi}\sum_{j\neq i}(J_x^{ij} - J_z^{ij})$. As a result, the ground-state pair discord in all these systems is finite and independent of pair separation or coupling range in the vicinity of B_s and given by Eqs. (21) or (24), with the values from Eqs. (29)–(33). Similar arguments apply in the vicinity of more general factorizing fields [26].

An example is provided in Fig. 6, where results for a fully and uniformly connected XY array (Lipkin-Meshkov-Glick (LMG) model [38]),

$$J_\mu^{ij} = (1 - \delta_{ij})J_\mu/(n-1), \quad \mu = x,y, \tag{35}$$

with the same anisotropy $J_y/J_x = 0.5$, are depicted. The exact result can be obtained here by direct diagonalization, as H can be expressed in terms of the total spin operators $S_\mu = \sum_i s_{i\mu}$. The reduced pair density is obviously independent of separation at any field. The pairwise entanglement is then small for large n, with a $O(n^{-1})$ concurrence [24].

The discord is, however, non-negligible and practically n-independent for large n. It is verified in Fig. 6 that, at $B = B_s$, the same previous limit (21) ($n = 100$) and side limits (24)–(33) ($n = 10$) at B_s are obtained. Moreover, the simple models (18) (large n) or (22) (small n) for the reduced density of a spin pair accurately describe the discord in the *whole region* $|B| < B_c = J_x$ (and not just at B_s) if the mean-field value $\cos\theta = B/J_x$ is employed for θ, as seen in Fig. 6. This indicates that the effects on D of correlations beyond the basic mean-field description with parity restoration of the ground state given by Eq. (30) become very small in this system, being negligible for large n. In contrast, such a mean-field model cannot accurately describe the pair discord (either for small or large separations) in the nearest-neighbor chain away from B_s.

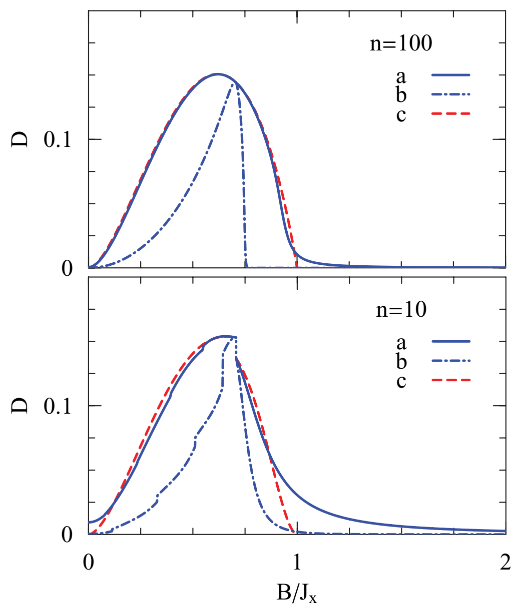

FIG. 6. (Color online) (top) Discord between spin pairs in the $n = 100$ fully connected array (a), together with the discord (21) of the state (18) at the mean-field angle $\cos\theta = B/J_x$ (c). The result for first-neighbor coupling at the same anisotropy and size n is also depicted (b) for large separation ($L = n/2$). The limits at the factorizing field B_s are exactly coincident. (bottom) Same details for $n = 10$ spins. Curve (c) depicts the result (24) for the actual mixture (22), which includes the coherence term. Side limits at B_s are again coincident.

IV. CONCLUSIONS

We have first discussed in detail the discord of a mixture of aligned pairs in two different directions. While exhibiting no entanglement if coherence effects between both directions are negligible, these mixtures do exhibit a finite and non-negligible quantum discord if the directions are neither coincident nor opposite. In the presence of coherence terms, however, entanglement becomes finite and can be larger than the discord.

Such mixtures become of crucial importance for studying the pair discord in the exact (and hence of definite parity) ground state of finite XY and XYZ spin chains in a transverse field. They represent the actual reduced state of an arbitrary pair in the vicinity of the factorizing field B_s. Previous results imply a finite discord between *any* two spins in the vicinity of B_s, irrespective of pair separation or coupling range. These mixtures are also the main term of the reduced pair state in the whole region $|B| < B_c$, implying a non-negligible pair discord even for pairs not linked by the couplings, as was seen in the nearest-neighbor case. Such mixtures do in fact accurately describe the pair discord $\forall\ |B| < B_c$ in the fully connected XY model.

The behavior of the discord, which is free from the monogamy restriction, differs then considerably from that of the pairwise entanglement, whose limits at B_s are small and determined by the coherence term. This term gives rise to a parity splitting and hence to a finite discontinuity of the discord at B_s, visible in small chains.

A final remark is that the present results, together with those previously obtained for the entanglement [24], allow us to identify the factorizing field as a quantum critical point for the ground state of an XY or XYZ chain of small size: At B_s, the last ground-state parity transition takes place and, in its immediate vicinity, pair quantum correlations as measured by the discord become independent of both pair separation and coupling range.

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APPENDIX: EXACT SOLUTION OF THE FINITE CYCLIC *XY* CHAIN

The Jordan-Wigner transformation [36] allows us to rewrite Eq. (3) for the case of first-neighbor couplings (26) and for each value ($\pm$) of the spin-parity P_z [Eq. (4)] as a quadratic form in fermion operators $c_i^\dagger$, c_i defined by $c_i^\dagger = s_{i+}\exp[-i\pi\sum_{j=1}^{i-1} s_{j+}s_{j-}]$:

$$\begin{aligned}H^\pm &= \sum_{i=1}^{n} B\left(c_i^\dagger c_i - \frac{1}{2}\right)\\ &\quad - \frac{1}{2}\eta_i^\pm(J_+ c_i^\dagger c_{i+1} + J_- c_i^\dagger c_{i+1}^\dagger + \text{H.c.})\\ &= \sum_{k\in K_\pm}\lambda_k\left(a_k^\dagger a_k - \frac{1}{2}\right),\end{aligned} \tag{A1}$$

where $J_\pm = \frac{1}{2}(J_x \pm J_y)$ and, in the cyclic case $n+1 \equiv 1$, $\eta_i^- = 1$, $\eta_i^+ = 1 - 2\delta_{in}$ [36]. In Eq. (A1),

$$\lambda_k^2 = (B - J_+\cos\omega_k)^2 + J_-^2\sin^2\omega_k, \quad \omega_k = 2\pi k/n,$$

with $K_+ = \{\frac{1}{2},\ldots,n-\frac{1}{2}\}$, $K_- = \{0,\ldots,n-1\}$, that is, k is a half-integer (integer) for positive (negative) parity [24,37]. The diagonal form of Eq. (A1) is obtained through a discrete *parity-dependent* Fourier transform $c_j^\dagger = \frac{e^{i\pi/4}}{\sqrt{n}}\sum_{k\in K_\pm} e^{-i\omega_k j} c_k'^\dagger$, followed by a BCS transformation $c_k'^\dagger = u_k a_k^\dagger + v_k a_{n-k}$, $c_{n-k}' = u_k a_{n-k} - v_k a_k^\dagger$ to quasiparticle fermion operators a_k, $a_k^\dagger$, with $u_k^2, v_k^2 = \frac{1}{2}[1 \pm (B - J_+\cos\omega_k)/\lambda_k]$. For $B \geqslant 0$, we set $\lambda_k \geqslant 0$ for $k \neq 0$ and $\lambda_0 = J_+ - B$ such that the quasiparticle vacuum in H^- is odd and the lowest energies for each parity are $E^\pm = -\frac{1}{2}\sum_{k\in k_\pm}\lambda_k$. At $B = B_s = \sqrt{J_x J_y}$, $\lambda_k = J_+ - B_s\cos\omega_k$ and $E^\pm = -nJ_+/2$ [24].

The concurrences in the fixed parity ground state can be obtained from the contractions $f_l \equiv \langle c_i^\dagger c_j\rangle_\pm - \frac{1}{2}\delta_{ij}$, $g_l \equiv \langle c_i^\dagger c_j^\dagger\rangle_\pm$ ($l = |i-j|$) and the use of Wick's theorem [36], leading to $\langle s_{iz}\rangle = f_0$, $\langle s_{iz}s_{jz}\rangle = f_0^2 - f_l^2 + g_l^2$, and $\langle s_{i-}s_{j\mp}\rangle = \frac{1}{4}[\det(A_l^+) \mp \det(A_l^-)]$, with $(A_l^\pm)_{ij} = 2(f_{i-j\pm1} + g_{i-j\pm1})$ $l\times l$ matrices. All previous results have been explicitly checked for small n with those obtained from a direct diagonalization.

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