Separability conditions and limit temperatures for entanglement detection in two-qubit Heisenberg *XYZ* models

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We examine the entanglement of general mixed states of a two-qubit Heisenberg *XYZ* chain in the presence of a magnetic field, and its detection by means of different criteria. Both the exact separability conditions and the weaker conditions implied by the disorder and the von Neumann entropic criteria are analyzed. The ensuing limit temperatures for entanglement in thermal states of different *XYZ* models are then examined and compared with the limit temperature of the symmetry-breaking solution in a mean-field-type approximation. The latter, though generally lower, can also be higher than the exact limit temperature for entanglement in certain cases, indicating that symmetry breaking does not necessarily entail entanglement. The reentry of entanglement for increasing temperatures is also discussed.

I. INTRODUCTION

Entanglement is one of the most distinctive features of quantum mechanics, representing the ability of composite quantum systems to exhibit correlations which have no classical analog. Recognized already by Schrödinger [1], it has recently become the object of intensive research due to the key role it plays in the field of quantum information [2–6]. Rigorously, a mixed state ρ of a bipartite system is said to be *separable* or *classically correlated* [7] if it can be expressed as a convex combination of uncorrelated densities, i.e., $\rho = \Sigma_\nu q_\nu \rho_A^\nu \otimes \rho_B^\nu$, where ρ_A^ν, ρ_B^ν are mixed states of each subsystem and q_ν are *non-negative* numbers. Otherwise, ρ is *entangled* or inseparable. When separable, ρ satisfies all Bell inequalities as well as other properties characteristic of classical systems.

A pure state $\rho = |\Phi\rangle\langle\Phi|$ is separable just for tensor product states $|\Phi\rangle = |\phi_A\rangle|\phi_B\rangle$, but in the case of mixed states, such as thermal states $\rho \propto \exp[-H/T]$, with H the system Hamiltonian, it is in general much more difficult to determine whether ρ is separable or not. Only in special cases, such as a two-qubit or qubit+qutrit system, simple necessary and sufficient conditions for separability are known [8,9]. Moreover, the entanglement of formation of a mixed state [10] has been explicitly quantified only for a two-qubit system [11]. Nonetheless, it is known that any mixed state becomes separable if it is sufficiently close to the fully mixed state [12,13]. For thermal states of finite systems, this implies that a *finite* limit temperature for entanglement [14], T_e, will always exist such that ρ becomes separable $\forall T \geq T_e$. It is then interesting to analyze if it is possible to estimate this temperature with simple separability criteria, and how it is related to the critical temperature T_c of the *symmetry-breaking* solution in a mean-field-type approximation, which is the conventional starting point for describing interacting many-body systems. Such solutions (i.e., like deformed or superconducting) normally reflect the presence of strong correlations and collective behavior.

The aim of this work is to examine these issues in a simple yet nontrivial model where the exact entanglement conditions and quantification can be easily obtained. For this purpose, we will consider a system of two qubits interacting through a Heisenberg *XYZ* Hamiltonian [15] in the presence of an external magnetic field. Interest in this model stems from the potential use of Heisenberg spin chains for gate operations in solid-state quantum computers [16,17]. The pairwise entanglement of thermal states of isotropic [18,19] and anisotropic *XY* [20–22] Heisenberg models have accordingly been recently studied, and several interesting features have appeared already in the two-qubit case [21], such as the possibility of entanglement reentry for increasing temperatures or magnetic fields.

We will first review the exact separability conditions for *general* mixtures of the eigenstates of arbitrary *XYZ* Hamiltonians, examining in particular thermal states and the possibility of entanglement reentry. We will also analyze the weaker conditions provided by the *disorder* criterion [23], which is the strongest one based just on the spectrum of ρ and one of its reductions, and is hence more easy to implement in general than other criteria. Violation of the disorder conditions also ensures distillability [24]. These conditions are here *exact* in the absence of a magnetic field. Although the disorder criterion admits a generalized entropic formulation [25], it is stronger than the von Neumann entropic criterion [26], based on the same information, whose predictions will also be analyzed. The ensuing exact and approximate limit temperatures for entanglement in thermal states of different *XYZ* models will then be examined.

Finally, we will discuss the mean-field (i.e., independent qubit) approximation for thermal states, with the aim of comparing the previous limit temperatures with the corresponding mean-field critical temperature T_c. It will be shown, remarkably, that for $T > 0$, *symmetry breaking is not necessarily a signature of entanglement*, so that T_c may be *higher* than T_e, although it is usually lower. The model and methods are described in Sec. II, while three different examples are analyzed in detail in Sec. III. Conclusions are finally drawn in Sec. IV.

II. FORMALISM

A. Model and separability conditions

We will consider a Heisenberg *XYZ* chain [15] for two qubits in an external magnetic field b along the z axis. Denoting with $S = s^A + s^B$ the total spin of the system, the corresponding Hamiltonian can be written as

$$H = bS_z - 2 \sum_{i=x,y,z} v_i s_i^A s_i^B, \qquad (1a)$$

$$= H_z - v_+(S_x^2 + S_y^2 - 1) - v_-(S_x^2 - S_y^2), \qquad (1b)$$

where $H_z = bS_z - v_z(S_z^2 - 1/2)$ and $v_\pm = (v_x \pm v_y)/2$. The ferromagnetic (antiferromagnetic) case corresponds to $v_i \geq 0$ (≤ 0), and the standard *XY* model to $v_z = 0$. Its normalized eigenstates $H|\Phi_j\rangle = E_j|\Phi_j\rangle$ are given by

$$|\Phi_{0,3}\rangle = \frac{|+-\rangle \mp |-+\rangle}{\sqrt{2}}, \quad E_{0,3} = \frac{1}{2}v_z \pm v_+,$$

$$|\Phi_{1,2}\rangle = \frac{u_\pm|++\rangle \mp u_\mp|--\rangle}{\sqrt{2}}, \quad E_{1,2} = -\frac{1}{2}v_z \pm \Delta, \qquad (2)$$

with $\Delta = v_-\sqrt{1 + b^2/v_-^2}$, $u_\pm = \sqrt{1 \pm b/\Delta}$ and $|\pm\pm\rangle \equiv |\pm\rangle|\pm\rangle$ the separable eigenstates of S_z (standard basis). The states $|\Phi_{0,3}\rangle$ are maximally entangled, whereas $|\Phi_{1,2}\rangle$ are entangled for $v_- \neq 0$, with concurrence v_-/Δ (see the Appendix). They become maximally entangled for $b = 0$, in which case the set of states (2) is just the Bell basis.

We will first consider general statistical mixtures of the previous eigenstates, which can be written as

$$\rho = \sum_{j=0}^{3} p_j |\Phi_j\rangle\langle\Phi_j| \qquad (3a)$$

$$= \frac{1}{4} + \frac{1}{2}\langle S_z\rangle S_z + 4 \sum_{i=x,y,z} \langle s_i^A s_i^B\rangle s_i^A s_i^B, \qquad (3b)$$

where $p_j \geq 0$, $\Sigma_{j=0}^{3} p_j = 1$ and

$$\langle S_z\rangle = \frac{b}{\Delta}(p_1 - p_2), \quad \langle s_z^A s_z^B\rangle = \frac{1}{2}\left(p_1 + p_2 - \frac{1}{2}\right),$$

$$\langle s_i^A s_i^B\rangle = \frac{1}{4}\left[p_3 - p_0 \pm \frac{v_-}{\Delta}(p_2 - p_1)\right], \quad i = x, y, \qquad (4)$$

with $\langle O\rangle \equiv \mathrm{Tr}\rho O$. Equations (3) comprise standard thermal states as well as those arising in more general statistical descriptions [27,28], and represent the most general two-qubit state with good permutational and phase flip symmetry $U = -e^{i\pi S_z}$ real in the standard basis. The two-site density matrix of an N qubit *XYZ* chain with cyclic boundary conditions is in fact also of this form [22].

Exact separability conditions. For the state (3), they can be most easily determined with the Peres criterion [8], sufficient for two qubits [9], and can be cast as

$$\frac{v_-}{\Delta}|p_2 - p_1| \leq p_0 + p_3, \qquad (5a)$$

$$|p_3 - p_0| \leq \left[(p_1 + p_2)^2 - \frac{b^2}{\Delta^2}(p_2 - p_1)^2\right]^{1/2}, \qquad (5b)$$

or, in terms of the averages $\langle S_i^2\rangle = 2\langle s_i^A s_i^B\rangle + 1/2$, as

$$|\langle S_x^2 - S_y^2\rangle| \leq \langle 1 - S_z^2\rangle, \qquad (6a)$$

$$|\langle S_x^2 + S_y^2 - 1\rangle| \leq [\langle S_z^2\rangle^2 - \langle S_z\rangle^2]^{1/2}, \qquad (6b)$$

imposing bounds on the averages of the last two terms in Eqs. (1b). If ρ is entangled, only one of Eqs. (5) is violated, and its concurrence is given precisely by the difference between the left- and right-hand sides of the broken inequality (see the Appendix). The entanglement arises essentially from one of the states $|\Phi_{1,2}\rangle$ ($|\Phi_{0,3}\rangle$) if Eq. (5a) [Eq. (5b)] is broken. Equations (5) are always satisfied if $|p_j - 1/4| \leq (4\sqrt{2})^{-1} \forall j$, i.e., if ρ is sufficiently close to the fully mixed state. If $b = 0$, ρ is diagonal in the Bell basis and Eqs. (5) reduce accordingly to $p_j \leq 1/2 \forall j$ [26], while Eqs. (6) to $1 \leq \langle S^2\rangle \leq 1 + 2\langle S_i^2\rangle$ for $i = x, y, z$, as $\langle S_z\rangle = 0$.

Disorder and entropic separability conditions. The disorder criterion [23] states that if ρ is separable, ρ is majorized by the reduced densities $\rho_{A,B} \equiv \mathrm{Tr}_{B,A} \rho$, which means that ρ is *more mixed* (i.e., *disordered*) than ρ_A, ρ_B. In a two-qubit system, this implies that the largest eigenvalue of ρ should not exceed that of ρ_A and ρ_B, which is in general a necessary condition that becomes *sufficient* when ρ is pure or *diagonal* in the Bell basis [23,25].

For the state (3), $\rho_\alpha = 1/2 + \langle S_z\rangle s_z^\alpha$ for $\alpha = A, B$, and the disorder criterion leads to the inequalities

$$p_j \leq \frac{1}{2}\left[1 + \left|\frac{b}{\Delta}(p_2 - p_1)\right|\right], \quad j = 0, \ldots, 3, \qquad (7)$$

which in terms of total spin averages can be recast as

$$|\langle S_x^2 - S_y^2\rangle| \leq \langle 1 - S_z^2\rangle[1 + 2|\langle S_z\rangle|/\langle 1 - S_z^2\rangle]^{1/2}, \qquad (8a)$$

$$|\langle S_x^2 + S_y^2 - 1\rangle| \leq \langle S_z^2\rangle + \langle S_z\rangle. \qquad (8b)$$

Equations (7) and (8) are clearly less stringent in general than Eqs. (5) and (6), but become *exact* for $b = 0$ ($\langle S_z\rangle = 0$), i.e., when ρ is diagonal in the Bell basis.

The standard entropic criterion [26], based on the von Neumann entropy $S_2(\rho) = -\mathrm{Tr}\,\rho\log_2\rho$, states that if ρ is separable, $S_2(\rho) \geq S_2(\rho_\alpha)$ for $\alpha = A, B$. Although exact for pure states [in which case $S_2(\rho) = 0$ and $S_2(\rho_A) = S_2(\rho_B)$ is just the entanglement of ρ [11]], for mixed states it is in general weaker than the disorder criterion [25], except when both ρ and ρ_α have rank two. Figure 1 depicts, for $p_1 = 0$ and $b/v_- = 1$, the regions where the state (3) is entangled and where entanglement is detected by the disorder and the standard entropic criteria.

Standard thermal state and entanglement reentry. For

FIG. 1. Range of values of p_2 and p_3 where the state (3) is entangled (shaded sectors), for $p_1=0$, $b/v_-=1$. Equation (5a) is broken in sector A while Eq. (5b) in sectors B. Entanglement is detected by the disorder criterion in the black and dark gray sectors, and by the von Neumann entropic criterion just in the black sectors. They both coincide at the border of the triangle, where ρ has rank 2, and are exact for $p_2=0$, where ρ is in addition diagonal in the Bell basis.

$$\rho = \exp[-\beta H]/\text{Tr} \exp[-\beta H], \quad \beta \equiv 1/T > 0, \quad (9)$$

i.e., $p_j \propto e^{-\beta E_j}$ in Eq. (3a), Eqs. (5) become

$$\frac{v_-}{\Delta}e^{\beta v_z}\sinh|\beta\Delta| \leq \cosh(\beta v_+), \quad (10a)$$

$$e^{-\beta v_z}\sinh|\beta v_+| \leq \left[1 + \frac{v_-^2}{\Delta^2}\sinh^2(\beta\Delta)\right]^{1/2}, \quad (10b)$$

and determine a finite limit temperature for entanglement T_e, such that they are satisfied $\forall T \geq T_e$. Nonetheless, entanglement, as measured by the entanglement of formation or concurrence, may not be a decreasing function of T for $T < T_e$ when the ground state is less entangled than the first excited state [18–21], and even entanglement vanishing plus reentry may occur [21], as discussed below. Note that the spectrum of H, and hence Eqs. (10), do not depend on the signs of b and $v_\pm$.

Let us consider for instance a mixture of $|\Phi_2\rangle$ and $|\Phi_3\rangle$ [$p_0=p_1=0$ in (3a)], which corresponds to the outer border in Fig. 1. This state is separable *just for* $p_2=p_c\equiv(1+v_-/\Delta)^{-1} \geq 1/2$, with Eq. (5a) [Eq. (5b)] broken for $p_2>p_c$ ($p_2<p_c$). Its concurrence is $C(\rho)=|p_2/p_c-1|$. The state (9) will approximately be of this form for low T if E_2 and E_3 are sufficiently close and well below the remaining levels. Hence, if $E_2 < E_3$, $C(\rho)$ will initially decrease as T increases from zero, *vanishing* at the temperature

$$T_r = (E_3 - E_2)/\ln[\Delta/v_-], \quad (11)$$

where $p_2=p_c$, but will exhibit a *reentry* for $T>T_r$, with Eq. (10a) [Eq. (10b)] broken for $T<T_r$ ($T_r<T<T_e$). Due to the remaining levels, $C(\rho)$ will actually vanish in a small but

finite temperature interval around T_r (see case 3 in Sec. III). When $|\Phi_2\rangle$ becomes separable ($v_-/b\to 0$), $p_c\to 1$ and $T_r \to 0$, whereas when it becomes maximally entangled ($b/v_- \to 0$), $p_c\to 1/2$ and $T_r\to\infty$, so that no reentry takes place in this limit. In contrast, if $E_3 < E_2$, $p_2 < 1/2 \leq p_c \ \forall \ T \geq 0$ and no reentry or enhancement of $C(\rho)$ can take place. Nor can it occur for a mixture of $|\Phi_0\rangle$ and $|\Phi_3\rangle$ or $|\Phi_1\rangle$ and $|\Phi_2\rangle$, since they are separable just for equal weights, as seen from Eqs. (5).

For the state (9), the disorder conditions (7) become

$$\left(1 - \left|\frac{b}{\Delta}\right|\right)e^{\beta v_z}\sinh|\beta\Delta| \leq \cosh(\beta v_+), \quad (12a)$$

$$e^{-\beta v_z}\sinh|\beta v_+| \leq \cosh(\beta\Delta) + \left|\frac{b}{\Delta}\right|\sinh|\beta\Delta|, \quad (12b)$$

and lead to a lower limit temperature for entanglement detection, $T_e^d \leq T_e$, with $T_e^d=T_e$ just for $b=0$. The entropic criterion leads to an even lower limit temperature $T_e^s \leq T_e^d$. The reentry effect *cannot be detected* by the disorder (and hence by the entropic) criterion. Violation of Eqs. (7) requires $p_j > 1/2$ for some j, so that in the thermal case just the entanglement arising from the *ground* state can be detected. For a mixture of $|\Phi_2\rangle$ and $|\Phi_3\rangle$, Eqs. (7) are broken just for $p_2 > p_d = (2-|b/\Delta|)^{-1}$ or $p_2 < p_d' = (2+|b/\Delta|)^{-1}$ (see Fig. 1), which does not allow to detect the reentry when $E_2 < E_3$ since $p_d' \leq 1/2$.

B. Symmetry-breaking mean-field approximation

The thermal state (9) represents the density operator that minimizes the free energy

$$F(\rho) \equiv \langle H \rangle - TS(\rho) = \text{Tr}\rho[H + T \ln \rho]. \quad (13)$$

In a finite temperature mean-field or independent qubit approximation, Eq. (13) is minimized among the subset of *uncorrelated* trial densities, given in this case by

$$\rho_{\text{mf}} = \rho_A \otimes \rho_B, \quad (14)$$

with arbitrary ρ_A, ρ_B, obtaining thus an upper bound to the minimum free energy. The only way such an approximation can reflect entanglement is through *symmetry breaking*: the optimum density that minimizes $F(\rho_{\text{mf}})$ may break some of the symmetries present in the Hamiltonian H, and become degenerate. In these cases a *critical temperature* T_c will exist such that the optimum density becomes symmetry conserving for $T \geq T_c$. At $T=0$, *symmetry breaking implies entanglement* if the ground state of H is nondegenerate, since for pure states separability corresponds to an uncorrelated density. However, this is not necessarily the case for $T>0$, where symmetry breaking just indicates, in principle, that the true thermal state is not uncorrelated. On the other hand, entanglement does not necessarily imply symmetry breaking either, both at $T=0$ or $T>0$, as correlations need to be in general sufficiently strong to induce a symmetry-breaking mean field [29].

The densities ρ_α, $\alpha=A, B$, can be parametrized as

$$\rho_\alpha = \frac{\exp[-\beta \boldsymbol{\lambda}^\alpha s^\alpha]}{\mathrm{Tr}\,\exp[-\beta \boldsymbol{\lambda}^\alpha s^\alpha]} = \frac{1}{2} + 2\langle s^\alpha \rangle s^\alpha,$$

$$\langle s^\alpha \rangle = \mathrm{Tr}\rho_\alpha\, s^\alpha = -\frac{1}{2}\boldsymbol{\lambda}^\alpha \tanh\left[\frac{1}{2}\beta|\boldsymbol{\lambda}^\alpha|\right] \Big/ |\boldsymbol{\lambda}^\alpha|, \quad (15)$$

so that Eq. (14) corresponds to an approximate independent qubit Hamiltonian $h = \Sigma_\alpha \boldsymbol{\lambda}^\alpha s^\alpha$. Minimization of $F(\rho_{\mathrm{mf}})$ with respect to $\boldsymbol{\lambda}^\alpha$ leads then to the self-consistent equations (see for instance Ref. [30])

$$\lambda_i^\alpha = \frac{\partial \langle H \rangle_{\mathrm{mf}}}{\partial \langle s_i^\alpha \rangle}, \quad i = x, y, z, \quad (16)$$

where $\langle H \rangle_{\mathrm{mf}} = \mathrm{Tr}\,\rho_{\mathrm{mf}} H$. A similar equation obviously holds for the n qubit case. In the case of Eq. (1), $\langle H \rangle_{\mathrm{mf}} = b\langle S_z \rangle - 2\Sigma_i\, v_i\langle s_i^A \rangle\langle s_i^B \rangle$ and Eqs. (16) become

$$\lambda_i^{A,B} = b\delta_{iz} - 2v_i\langle s_i^{B,A} \rangle. \quad (17)$$

Permutational symmetry will be broken if $\boldsymbol{\lambda}^A \neq \boldsymbol{\lambda}^B$, and phase flip symmetry if $\lambda_x^\alpha \neq 0$ or $\lambda_y^\alpha \neq 0$. The latter has to be broken in order to see any effect from the last two interaction terms in Eq. (1b) at the mean-field level, since otherwise their mean-field averages vanish. In such a case the sign of one of the λ_x^α (or λ_y^α) remains undetermined, giving rise at least to a two-fold degeneracy.

For instance, in the ferromagnetic case $v_i \geq 0$, $\langle H \rangle_{\mathrm{mf}}$ is minimum for $\langle \mathbf{s}^A \rangle = \langle \mathbf{s}^B \rangle$ and permutational symmetry need not be broken. Hence, $\boldsymbol{\lambda}^{A,B} = \boldsymbol{\lambda}$. Defining $v_M = \mathrm{Max}[v_x, v_y]$, $v_m = \mathrm{Min}[v_x, v_y]$, a phase-flip symmetry breaking solution with $|\lambda_M| \neq 0$ and $\lambda_m = 0$ becomes feasible and provides the lowest free energy if $v_M > v_z$ and $|b| < b_c \equiv v_M - v_z$, provided $0 \leq T < T_c$, with

$$T_c = v_M \chi / \ln\left[\frac{1+\chi}{1-\chi}\right], \quad \chi \equiv |b|/b_c < 1. \quad (18)$$

T_c decreases as χ increases, with $T_c \to 0$ for $\chi \to 1$ and $T_c \approx \frac{1}{2}v_M(1 - \chi^2/3)$ for $\chi \ll 1$. This solution is insensitive to v_m. As discussed in Sec. III, T_c is usually lower than T_e, but can also be *higher*. For example, if $b = 0$ and $v_x > v_y = v_z > 0$, $T_c = v_x/2$, but the ensuing exact thermal state, diagonal in the Bell basis, is *separable* $\forall T > 0$ ($T_e = 0$), as the ground state is degenerate ($E_2 = E_3 = -v_x/2$) and hence $p_j \leq 1/2 \ \forall \ j, T$.

III. EXAMPLES

We now examine in detail the previous limit temperatures in three different cases. We set in what follows $b \geq 0$, $v_\pm \geq 0$, since the concurrence and limit temperatures are independent of their signs.

1) $v_- = 0$, $v_+ > 0$ (*XXZ* model). The states $|\Phi_{1,2}\rangle$ are in this case *separable*, with $\Delta = b$ in Eq. (2). Entanglement can then only arise through the violation of Eq. (5b), i.e., Eq. (10b) in the thermal case, which is now *independent* of the magnetic field b. If $v_+ > v_z$, the thermal state (9) will then be entangled for *any* b if $T > 0$, up to a limit temperature T_e that is independent of b. However, the ground state is $|\Phi_3\rangle$ if $b < b_0$
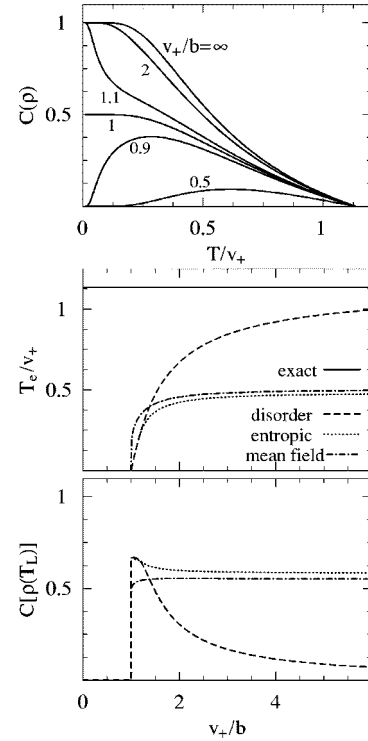

FIG. 2. Top: the concurrence as a function of temperature for $v_- = v_z = 0$ and indicated values of v_+/b. Center: The corresponding exact limit temperature for entanglement (constant) and the limit temperatures below which entanglement is detected by the disorder and by the von Neumann entropic criterion. The critical temperature for the symmetry-breaking mean-field approximation is also shown. Bottom: the concurrence at the previous limit temperatures.

$\equiv v_+ - v_z$ and $|\Phi_2\rangle$ if $b > b_0$, so that for $b > b_0$, ρ becomes entangled only at *finite temperature* $T > 0$, in agreement with Eq. (11) ($T_r \to 0$ for $v_-/b \to 0$). On the other hand, if $v_+ < v_z$, no entanglement occurs at any temperature. These features can be appreciated in Fig. 2 for $v_z = 0$ (*XX* model), where $b_0 = v_+$ and [20]

$$T_e = \alpha v_+, \quad \alpha = 1/\ln[1 + \sqrt{2}] \approx 1.134. \quad (19)$$

The disorder criterion can now detect entanglement just through the violation of Eq. (7) for $j = 0, 3$, i.e., Eq. (12b) in the thermal case, which can occur only for $b < b_0$, i.e., when $|\Phi_3\rangle$ is the ground state. The entanglement arising for $T > 0$ when $b > b_0$ cannot be detected. In addition, the limit temperature T_e^d determined by Eq. (12b) will depend on b, decreasing as b increases and vanishing for $b \to b_0$. Its behavior for $v_z = 0$ is shown in the central panel of Fig. 2, where $T_e^d \approx T_e[1 - b/(\sqrt{2}v_+)]$ for $b \to 0$ while $T_e^d \approx (v_+ - b)/\ln 2$ for $b \to b_0 = v_+$. Also shown is the concurrence at $T = T_e^d$ (bottom panel), which is maximum at $b = b_c$ [where $C(\rho(T_e^d)) \to 2/3$] and decreases as $\approx \alpha^{-1}(\sqrt{2} - 1)b/v_+$ for $b \to 0$. The limit temperature T_e^s of the entropic criterion is still lower. For $v_z = 0$ and $b \to 0$, $T_e^s \to 0.478v_+$, with $C(\rho(T_e^s)) \to 0.584$.

In this case the ground-state critical field b_0 *coincides* with the mean-field critical field b_c. Hence, a stable symmetry breaking mean-field solution is here feasible just for
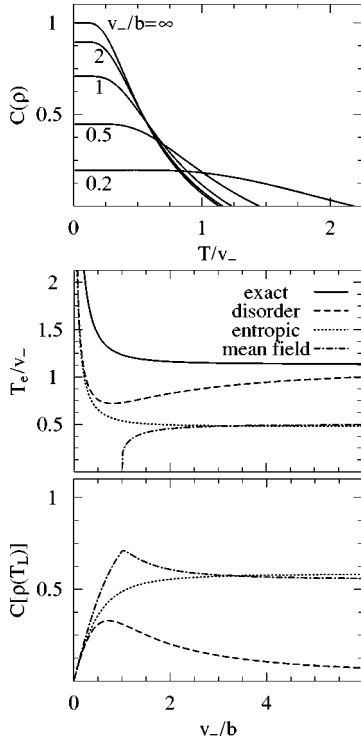
FIG. 3. Same quantities as in Fig. 2 for $v_+=v_z=0$ and different values of v_-/b.

$b<b_0$, with T_c given by Eq. (18) with $v_M=v_+$. Since now $[H,S_z]=0$, this "deformed" solution breaks the rotational invariance around the z axis and possesses, accordingly, a *continuous degeneracy*. As seen in Fig. 2, for $v_z=0$ T_c is *much lower* than T_e, lying actually quite close to the entropic limit temperature T_e^s. For $b\to0$, $T_c\to v_+/2$, with $C(\rho(T_c))\to0.55$. Note, however, that for $b\to b_0$, $T_c>T_e^d$ due to the logarithmic vanishing of T_c in this limit, where $C(\rho(T_c))\to1/2$.

2) $v_->0$, $v_+=0$. This case of maximum anisotropy ($v_x=-v_y$) represents, for $v_z=0$, the two-qubit version of the standard Lipkin model, widely employed in nuclear physics to test symmetry-breaking mean-field based descriptions [29]. It describes the interplay between a single-particle term bS_z and a monopole interaction that induces a deformed mean field. The states $|\Phi_{1,2}\rangle$ are now entangled, whereas the states $|\Phi_{0,3}\rangle$ become *degenerate*. Hence, in the thermal case $p_3=p_0$, and entanglement can only arise from the states $|\Phi_{1,2}\rangle$, i.e., through the violation of Eq. (5a) [Eq. (10a) in the thermal case]. This requires $\Delta>-v_z$, i.e., that $|\Phi_2\rangle$ be the ground state.

The limit temperature T_e determined by Eq. (10a) depends now on the field b, with ρ entangled for $0\leq T<T_e$ and $C(\rho)$ a decreasing function of T, as seen in Fig. 3 for $v_z=0$. In this case, entanglement occurs $\forall\,b$ and

$$T_e = \Delta/\mathrm{arcsinh}\left[\frac{\Delta}{v_-}\right], \qquad (20)$$

with $T_e\approx\alpha v_-[1+\frac{1}{2}(1-\alpha/\sqrt{2})b^2/v_-^2]$ for $b\to0$. A remarkable feature is that as b increases, T_e now *increases*, even though the entanglement of $|\Phi_2\rangle$ decreases, since the energy

gap Δ between the ground and the first excited states increases. Moreover, for $b\to\infty$, $T_e\approx b/\ln(2b/v_-)\to\infty$, being then possible to make ρ entangled at *any* temperature by increasing the field.

For $p_0=p_3$, entanglement will be detected by the disorder criterion through the violation of Eq. (7) for $j=1,2$, i.e., of Eq. (12a). For $v_z=0$, this will occur for any value of b but below the lower limit temperature

$$T_e^d = \Delta/\mathrm{arcsinh}\left[\frac{\Delta}{\Delta-b}\right]. \qquad (21)$$

For $b\to0$, $T_e^d\approx T_e[1-\alpha b/(\sqrt{2}v_-)]$, with $C(\rho(T_e^d))\approx(\sqrt{2}-1)b/v_-$. Equation (21) is not a monotonous increasing function of b, being minimum at $b\approx1.25v_-$, but for $b\to\infty$, $T_e^d\approx b/\ln[4b^2/v_-^2]\approx T_e/2$, becoming then also infinite in this limit. Hence, the emergence of entanglement for large fields is also detected (since it is a ground state effect) but above a higher threshold. Note also that $T_e^d/T_e\gtrless1/2\,\forall\,b$, with $C(\rho(T_e^d))\lesssim0.33$. The limit temperature of the entropic criterion lies very close to T_e^d for $b\to\infty$ (as $T_e^d/\Delta\to0$ in this limit) but becomes smaller as b decreases, with $T_e^s\to0.478v_-$ for $b\to0$.

For $v_z=0$, a phase flip symmetry breaking mean field solution becomes here feasible *only for* $b<b_c=v_-$. For $b>b_c$, ground-state correlations, though nonvanishing, are not strong enough to induce a symmetry-breaking mean field, so that the entanglement effect for large fields cannot be captured by the mean field. The permutationally invariant solution corresponds to $\lambda_x\neq0$ and $\lambda_y=0$, so that the critical temperature is given again by Eq. (18) with $v_M=v_-$. Hence, $T_c\to v_-/2$ for $b\to0$, lying again very close to T_e^s in this limit, while $T_c\to0$ for $b\to b_c$, where $C(\rho(T_c))\to1/\sqrt{2}\approx0.71$.

3) $v_+>0$, $v_->0$. This is the case with *finite* anisotropy $\gamma=v_-/v_+>0$, where entanglement vanishing plus reentry may occur as T increases. For $v_+>v_z\geq0$, the two lowest states are $|\Phi_2\rangle$ and $|\Phi_3\rangle$, with $E_2<E_3$ for $\Delta>v_+-v_z$, i.e., $b^2>b_0^2=\mathrm{Max}[0,(v_+-v_z)^2-v_-^2]$. For b above but close to b_0, Eq. (10a) [Eq. (10b)] will be broken for $0\leq T<T_r^-$ ($T_r^+<T<T_e$), with $T_r^-<T_r^+$. Hence, as T increases from zero, the concurrence will first decrease, *vanishing* for $T\in[T_r^-,T_r^+]$, but will exhibit a reentry for $T>T_r^+$, vanishing finally for $T\gtrsim T_e$.

This behavior is depicted in Fig. 4 for $v_z=0$ and $\gamma=0.7$, where $b_0\approx0.71v_+$ and the reentry occurs for $b_0<b<b_r\approx1.1v_+$. For b close to b_0, T_r^- and T_r^+ are practically coincident and equal to the value given by Eq. (11), $T_r=(\Delta-v_+)/\ln[\Delta/v_-]$, becoming the difference exponentially small for $b\to b_0$ ($T_r^+-T_r^-\approx T_r e^{-2v_+/T_r}$). For $b>b_r$ the reentry disappears and T_e becomes the continuation of T_r^-, undergoing then a sharp drop at $b=b_r$. For $b\to\infty$, $T_e\to\infty$, as in case 2, while for $b\to0$, $T_e\to0.93v_+$. At fixed $T<0.93v_+$, entanglement vanishing plus reentry will then also occur as b increases.

As discussed in Sec. II, the disorder criterion cannot detect the reentry for increasing T. Instead, the limit temperature T_e^d vanishes for $b\to b_0$, as seen in Fig. 4, with Eq. (12a) broken for $b>b_0$ and (12b) for $b<b_0$. Nevertheless, T_e^d
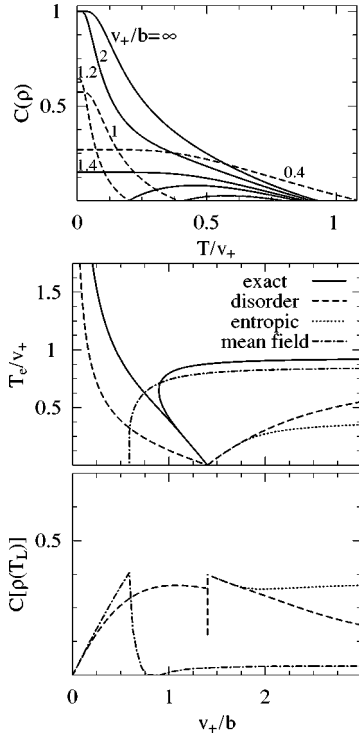
FIG. 4. Same quantities as in Fig. 2 for $v_+ > 0$ and finite aniso-tropy $\gamma = v_+/v_- = 0.7$. Entanglement vanishing plus reentry occurs as T increases for $0.9 \lesssim v_+/b \lesssim 1.4$, as indicated by the solid lines of the central panel. In the top panel, dashed (solid) lines depict the concurrence in the interval where Eq. (5a) [Eq. (5b)] is broken.

$\rightarrow T_e/2$ for $b \rightarrow \infty$, so that the entanglement effect for large fields will be detected, whereas $T_e^d \rightarrow T_e$ for $b \rightarrow 0$, with $T_e - T_e^d \propto b$ for $b \rightarrow 0$. Note also that T_e^s lies very close to T_e^d for $b \gtrsim 0.55 v_+$, but becomes lower as b decreases, with $T_e^s \rightarrow 0.39 v_+$ for $b \rightarrow 0$. Now $C(\rho(T_e^d)) < 0.37 \, \forall b$, with $C(\rho(T_e^d)) = 0.15$ for $b = b_0$ and $C(\rho(T_e^d)) \rightarrow 0.37$ and 0.32 for $b \rightarrow b_0^{\mp}$. This discontinuity arises from that of $C(\rho)$ for $T = 0$ [where $C(\rho) = 0.15$ at $b = b_c$ while $C(\rho) \rightarrow 1$ and 0.7 for $b \rightarrow b_0^{\mp}$, respectively].

For $v_z = 0$, a stable mean-field solution breaking phase flip symmetry becomes feasible only if $b < b_c = v_x$, with $v_x = v_+ + v_- > b_0$ and T_c given by Eq. (18) with $v_M = v_x$. The ratio T_c/v_+ is then larger than in case 1. For $\gamma = 0.7$, T_c lies close to T_e for $b \lesssim v_+$, with $T_c \rightarrow 0.85 v_+$ and $C(\rho(T_c)) \rightarrow 0.034$ for $b \rightarrow 0$. However, the most striking effect is that $T_c > T_e$ for $1.1 \lesssim b/v_+ \lesssim 1.33$, i.e., for b just above the reentry interval. In this region, ρ becomes separable at a low temperature, yet correlations remain strong to induce a symmetry-breaking mean field. On the other hand, for $b > b_c$ the ground state remains entangled but correlations are not strong enough to induce symmetry breaking, as occurs in case 2.

IV. CONCLUSIONS

We have examined the exact and the disorder separability conditions for general mixed states of two qubits interacting through a general *XYZ* Heisenberg Hamiltonian, which can be succinctly expressed in terms of total spin expectation

values. The disorder conditions are exact in the absence of a magnetic field, but become weaker as the field increases and are unable to detect the reentry of entanglement for increasing temperatures in thermal states, an effect which may here arise when the ground state is less entangled than the first excited state. The von Neumann entropic criterion leads to still lower limit temperatures and is not exact even for zero field. Nonetheless, both the disorder and entropic criteria do predict the increase in the limit temperature for large fields occurring in anisotropic models.

The critical temperature for the symmetry-breaking mean field solution is normally also lower than the exact limit temperature for entanglement in the examples considered and always vanishes for sufficiently large fields. However, it can also be higher, particularly when the lowest energy levels are close and entangled, implying that such solutions, normally regarded as signatures of the presence of strong correlations in the system, are not rigorous indicators of entanglement for $T > 0$. It is well known that in small systems, the sharp thermal mean-field transitions are to be interpreted just as rough indicators of a smooth crossover between two regimes. The concept of entanglement allows, however, to formulate a crossover precisely. Finite systems regain in this sense a critical-like behavior for increasing T, becoming classically correlated (but not uncorrelated) for $T \gtrsim T_e$, and with an entanglement undetectable through the eigenvalues of ρ and one of its reductions for $T_e^d \lesssim T < T_e$.

APPENDIX

The concurrence of a mixed state ρ of two qubits is a measure of the entanglement of ρ, given by Ref. [11]

$$C(\rho) = \text{Max}[2\lambda_M - \text{Tr } R, 0], \tag{A1}$$

where λ_M is the largest eigenvalue of $R = [\rho^{1/2} \tilde{\rho} \rho^{1/2}]^{1/2}$ and $\tilde{\rho}$ the spin-flipped density operator, given in the standard basis by $\tilde{\rho} = (\sigma_y \otimes \sigma_y) \rho^* (\sigma_y \otimes \sigma_y)$, with σ_y the Pauli matrix. The entanglement of formation [10] is an increasing function of $C(\rho)$ and can be obtained as

$$\mathcal{E}(\rho) = -\sum_{\nu=\pm} q_\nu \log_2 q_\nu, \quad q_\pm = \frac{1}{2}[1 \pm \sqrt{1 - C^2(\rho)}].$$

Maximum entanglement corresponds to $C(\rho) = 1$, separability to $C(\rho) = 0$. For a pure state $\rho = |\Phi\rangle\langle\Phi|$, $C(\rho) = |\langle\Phi|\tilde{\Phi}\rangle|$ and $\mathcal{E}(\rho)$ becomes the von Neumann entropy of the subsystems [11], $S_2(\rho_A) = S_2(\rho_B)$.

For the state (3), the eigenvalues of R are

$$\lambda_{1,2} = \frac{1}{2}\left\{\left[(p_1 + p_2)^2 - \frac{b^2}{\Delta^2}(p_2 - p_1)^2\right]^{1/2} \pm \frac{v_-}{\Delta}(p_1 - p_2)\right\},$$

and $\lambda_{0,3} = p_{0,3}$. Hence, if $\lambda_M = \lambda_1$ or λ_2 (λ_0 or λ_3), Eq. (A1)

becomes the difference between the left- and right-hand sides of Eq. (5a) [Eq. (5b)] when positive.

The eigenvalues of the partial transpose of Eq. (3) are $q_{1,2} = \frac{1}{2}[p_0 + p_3 \pm (v_- / \Delta)(p_2 - p_1)]$ and $q_{0,3} = \frac{1}{2}\{p_1 + p_2 \pm [(p_3 - p_0)^2 + (b^2 / \Delta^2)(p_2 - p_1)^2]^{1/2}\}$, so that the conditions $q_j \geq 0 \, \forall \, j$ also lead to Eqs. (5). Only one of them, q_m, is negative when ρ is entangled [31], with $q_m = \text{Min}[q_1, q_2]$ ($\text{Min}[q_0, q_3]$) if $\lambda_M = \lambda_1$ or λ_2 (λ_0 or λ_3). In the first case $C(\rho) = -2q_m$ but in the second case, $C(\rho) \neq -2q_m$ unless $b = 0$ or $p_1 = p_2$.

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