Enhancement of pairwise entanglement via $\mathbb{Z}_2$ symmetry breaking

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We study the effect of symmetry breaking in a quantum phase transition on pairwise entanglement in spin-1/2 models. We give a set of conditions on correlation functions a model has to meet in order to keep the pairwise entanglement unchanged by a parity symmetry breaking. It turns out that all mean-field solvable models do meet this requirement, whereas the presence of strong correlations leads to a violation of this condition. This results in an order-induced enhancement of entanglement, and we report on two examples where this takes place.

Entanglement is a non-locality inherent to quantum mechanics and an important resource for quantum optics and quantum information processing. It also has attained a lot of interest in the last decade from condensed matter physicists, especially since a connection between quantum non-locality and quantum phase transitions was proposed [1, 2]. This initiated a vast analysis of quantum critical models with respect to their entanglement features based on the few computable entanglement measures at hand [3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17]. One of the entanglement measures probed on such models is the concurrence [18, 19, 20], a measure of pairwise entanglement for spins-1/2 (qubits). Most of the results obtained in the literature make use of certain symmetries of the model Hamiltonian which reflect in the reduced density matrix. In presence of quantum phase transitions, a symmetry is typically broken in the *ordered* region with non-vanishing order parameter. The effect of the broken symmetry on the entanglement largely has not been taken into account in the existing literature (but see e.g. [2] for the local entropy). It was exactly this subject which has been addressed by Syljuåsen in [21, 22] for the quantum-Ising and the ferromagnetic XXZ model, where a parity symmetry is broken at the transition. He provided a condition on correlation functions that guarantees the invariance of the concurrence under symmetry breaking. The models under consideration there fulfill this condition. The focus of the present work is to investigate the regime where Syljuåsen's condition is violated as it happens for the XY model in transverse field.

In this letter, we first summarize the main result of Ref. [21]. Then, we derive the condition for two-point correlation functions and form factors that guarantees the invariance of the concurrence under parity symmetry breaking where the Syljuåsen condition does not apply. Finally, we illustrate our result, showing that mean-field solvable models satisfy this condition and demonstrating that symmetry breaking in general must be given account for, both for the XY spin chain in transverse magnetic field and the Lipkin-Meshkov-Glick (LMG) model.

We will next review the main result of Ref. 21, adopting for the sake of cross-readability the notation used in this work. The model Hamiltonians H under consideration have a parity symmetry or global phase flip symmetry, meaning that the eigenstates can be chosen as superpositions from states all having the same parity of flipped spins (i.e.: odd or even). It is reflected by $[\prod_i \sigma_i^z, H] = 0$. The general 2 sites density matrix of such a system is given by

$$\rho_{ij} = \begin{pmatrix} A & a & a & F \\ a & B & C & b \\ a & C & B & b \\ F & b & b & D \end{pmatrix}, \tag{1}$$

where indices for the entries of the density matrix have been omitted. The entries of ρ are related to spin correlators as follows: $a = (\langle S^x\rangle + 2\langle S^x S^z\rangle)/2$, $b = (\langle S^x\rangle - 2\langle S^x S^z\rangle)/2$, $A = \langle S^z S^z\rangle + \langle S^z\rangle + 1/4$, $B = 1/4 - \langle S^z S^z\rangle$, $C = \langle S^x S^x\rangle + \langle S^y S^y\rangle$, $D = \langle S^z S^z\rangle - \langle S^z\rangle + 1/4$ and $F = \langle S^x S^x\rangle - \langle S^y S^y\rangle$. The symmetry-breaking manifests itself in $a, b \neq 0$. For $a = b = 0$, the square root of the eigenvalues of $\rho\tilde{\rho}$ are $B \pm C$ and $\sqrt{AD} \pm F$. The concurrence of a 2-site reduced density matrix ρ is computed from the positive semidefinite matrix $R := \rho(\sigma_y \otimes \sigma_y)\rho^*(\sigma_y \otimes \sigma_y)$ as $\mathcal{C} = \max\{0, 2\lambda_{max} - \mathrm{tr}\,\sqrt{R}\}$, where λ_{max} is the maximum eigenvalue of $\sqrt{R}$. Thus the concurrence is $\mathcal{C} = 2\max\left\{0, |C| - \sqrt{AD}, |F| - B\right\} =: 2\max\{0, \mathcal{C}_{af}, \mathcal{C}_f\}$. We refer to the concurrence as belonging to the anti-ferro- or ferromagnetic sector whenever the largest eigenvalue of $\sqrt{R}$ is from this sector and denote it by $\mathcal{C}_{af}$ and $\mathcal{C}_f$, respectively. Throughout all the letter will we adopt the notation $\langle S^\alpha S^\beta\rangle := \left\langle S_i^\alpha S_j^\beta\right\rangle$ and $\langle S^z\rangle := (\langle S_i^z\rangle + \langle S_j^z\rangle)/2$. For the models considered here, the Hamiltonian is real and so is the density matrix.

In order to study the effect of symmetry breaking, accompanied by non-zero $\langle S^x S^z\rangle$ and order parameter $\langle S^x\rangle$, one has to extract the dependence of the eigenvalues of R on a and b. This task simplifies since the eigenvector $(0, 1, -1, 0)$ (the singlet Bell state) and its eigenvalue $B-C$ are unchanged. If $C>0$, this robust eigenvalue can not become the largest one.

The exact factoring of a cubic polynomial is not very handy and has been cleverly avoided by Syljuåsen, when concentrating on the coefficients of the characteristic polynomial $X^3-g_2X^2+g_1X-g_0$ of R with $g_0=(xyz)^2$, $g_1=x^2y^2+x^2z^2+y^2z^2$, and $g_2=x^2+y^2+z^2$ rather than studying the eigenvalues of $\sqrt{R}$ themselves. The connection between the g_i's and the entries of the reduced two-spin density matrix is [21]

$$g_0 = (\alpha^2-4\gamma\delta)\beta-4\mu\nu\alpha-4\mu^2\delta-4\nu^2\gamma \qquad (2)$$
$$g_1 = \alpha^2+2\alpha\beta-4\mu\nu-4\gamma\delta \qquad (3)$$
$$g_2 = 2\alpha+\beta \qquad (4)$$

where $\alpha=F^2+AD-2ab$, $\beta=(B+C)^2-4ab$, $\gamma=DF-b^2$, $\delta=AF-a^2$, $\mu=aD-b(B+C-F)$ and $\nu=a(B+C-F)-bA$. The concurrence would then simply be expressed as $\mathcal{C}=\max\{0,\kappa-(B-C)\}$, with $\kappa:=z-x-y$ and z the largest eigenvalue of $\sqrt{R}$. The condition that the concurrence be unaffected by symmetry breaking is then [21]

$$2\kappa\sqrt{g_0}=\left(\frac{\kappa^2-g_2}{2}\right)^2-g_1\ . \qquad (5)$$

Interestingly, for dominating $\mathcal{C}_f$, i.e. when $\sqrt{AD}+|F|$ is largest, this condition is identically satisfied which is the main outcome of Ref. [21].

We will now extend the analysis of Ref. [21] to the regime where $\mathcal{C}_{af}$ dominates, but still $C>0$. The case $C<0$ and $B-C$ being the largest eigenvalue of $\sqrt{R}$, is treated the same way, just replacing κ by $\tilde{\kappa}:=x+y+z$.

It is a generic feature of quantum spin models (with competing interactions) that there is a point in coupling parameter space at which the ground state factorizes [15, 23, 24]. At such a *factorizing field* any measure of entanglement must vanish. If at both sides of a factorizing point the concurrence is non-zero, there are two scenarii: either the concurrence is smooth at h_f or the sector giving support to the concurrence necessarily has to change at this point. It is the latter scenario which actually takes place in the models examined so far in the literature as e.g. the transverse XY model [1, 25], the XYZ model [15, 16], and the Lipkin-Meshkov-Glick model (LMG) [3, 26]; the Syljuåsen condition applies between the factorizing and the quantum critical field. The explicit form of the concurrence for parity symmetric models and translational symmetry (which includes all above cited studies) implies that $\mathcal{C}_{af}=\mathcal{C}_f=0$ at the factorizing field, and they cross unless $2\langle S^yS^y\rangle-(\langle S^zS^z\rangle-\langle S^z\rangle^2)/(2\langle S^x\rangle^2)\sim(h-h_f)^n$ with even $n>0$ (for symmetry breaking field in x-direction). If only one crossing occurs, then the concurrence is robust against $\mathbb{Z}_2$ symmetry breaking between critical and factorizing point. Below the factorizing field $\mathcal{C}_{af}$ dominates and the concurrence will in general be affected by the broken symmetry. Nonetheless, to the best of our knowledge no such case has been reported in the literature, which motivates the search for further conditions that make the concurrence robust against symmetry breaking or for examples where the concurrence *is* affected. We will show in this letter that both cases occur.

Having taken the square of Eq.(5) and inserted $\kappa\to B+C-2\sqrt{AD}$, the resulting expression is conveniently expressed in the new variables $\lambda:=b/a$ and a, leading to

$$32a^2(\lambda-\lambda_0)^2\left[1+a^2(\lambda-\lambda_1)(\lambda-\lambda_2)\right]=0\quad , \qquad (6)$$

where $\lambda_0=\sqrt{D/A}$, $\lambda_1+\lambda_2=2\kappa/A$ and $(\lambda_1-\lambda_2)^2=4\kappa(B+C)/A^2$.

Both λ_1 and λ_2 are real for $\kappa\geq 0$, which is mandatory for a non-vanishing concurrence. The real solutions to Eq. (6) are constraints on the correlation functions of the model which insure the concurrence to be unaffected by symmetry breaking. The solution $\lambda=\lambda_0$ can then be recast into a simple condition:

$$\frac{\sqrt{(1+4\langle S^zS^z\rangle)^2-16\langle S^z\rangle^2}}{1+4\langle S^z\rangle+4\langle S^zS^z\rangle}\equiv\frac{\langle S^x\rangle-2\langle S^xS^z\rangle}{\langle S^x\rangle+2\langle S^xS^z\rangle}\ . \qquad (7)$$

Note that this condition is automatically satisfied for mean-field solvable models as a direct consequence of the factorization of the two-point functions in this case.

Another real solution to Eq.(6) exists if $a\leq -1$ and

$$\langle S^x\rangle\left(\frac{\lambda_1-\lambda_2}{\lambda_1+\lambda_2+2}\right)^2=\pm\frac{1}{\pi} \qquad (8)$$

to insure the reality of both a and b. This leads to the following transcendental equation

$$\kappa\frac{B+C}{(\kappa+A)^2}\ln\left(\frac{\kappa}{A}|a|-1\right)=\frac{A(\kappa+A)}{A(\kappa+A)+2\kappa^2}\frac{1}{\pi|a|}\ . \qquad (9)$$

Eq. (9) has a unique real solution for arbitrary A, B and κ. The rewriting of this condition in terms of correlation function is lengthy but straightforward. There is numerical evidence that $a<-1$ only occurs for a two-site reduced density matrix of rank 3 or less. Interestingly, rank 3 and 2 are assumed for the (2-magnon) W state $\sum_i w_{ij}S_i^+S_j^+|\Downarrow\rangle$ and GHZ (cat) state $|\Downarrow\rangle+|\Uparrow\rangle$ of the whole chain, where $w_{ij}\in\mathbb{C}$ and $|\Uparrow\rangle$ and $|\Downarrow\rangle$ are in opposite direction fully polarized states. If Eqs. (7) and (8)–(9) are violated, the concurrence will be affected by symmetry-breaking, as condition (5) is then violated.

<u>LMG model</u> The LMG model [27] in transverse field is described by the Hamiltonian

$$H_{LMG}=-\frac{1}{N}\sum_{i<j}\left(\sigma_x^i\sigma_x^j+\gamma\sigma_y^i\sigma_y^j\right)-h\sum_i\sigma_z^i \qquad (10)$$

where the σ_α^i are the Pauli matrices for the i-th lattice site and N is the chain length. Any two spins are interacting with the same coupling strength. The prefactor $1/N$ leads to a finite free energy per spin in the thermodynamic limit. H commutes with the total spin and the spin-flip operator $\prod_i \sigma_z^i$ for any anisotropy parameter γ. This discrete $\mathbb{Z}_2$ symmetry is broken at the quantum critical point, $h_c = 1$. The factorizing field of this model is $h_f = \sqrt{\gamma}$. Due to its infinite-range coupling, the mean-field approximation for the LMG model becomes exact in the thermodynamic limit [28]. In this limit, condition (7) is satisfied for arbitrary transverse field. The non-trivial behavior of the entanglement of the LMG lies in the finite-size corrections to the mean-field solution [3, 26].

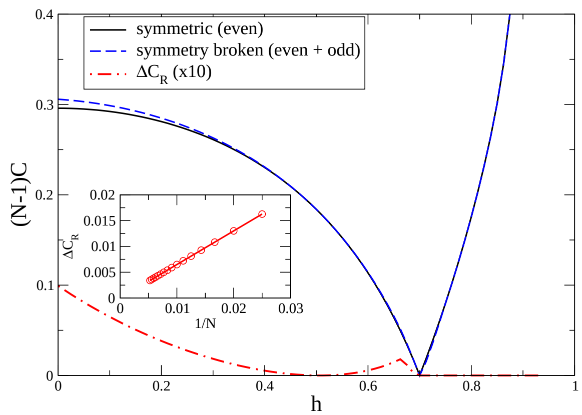

FIG. 1: Rescaled concurrence for the LMG model: The even sector (full line) and the symmetry broken (dashed line) concurrence is shown for $N = 100$ and $\gamma = 0.5$; the inset shows the difference between the rescaled concurrence in the $\mathbb{Z}_2$-symmetric case and in the $\mathbb{Z}_2$-broken case for fixed magnetic field $h = 0.2 < h_f$. It scales as $a_0/N + a_1$, with $a_0 = 0.651622$ and $a_1 \simeq 10^{-5}$. The dash-dotted curve is this difference rescaled by a factor of 10 as a function of the magnetic field. It goes to zero at $h \sim 0.5$. At such a point, one of the conditions for the correlation functions of the model must be satisfied.

In Fig. 1 we report numerical data for the rescaled concurrence, $\mathcal{C}_R = (N-1)\mathcal{C}$, for the even (black full curve) and $\mathbb{Z}_2$-broken (blue dashed curve) ground state. In the thermodynamic limit (N goes to ∞ while the free energy per spin remains finite), both curves coincide. The analytic expression of this limiting curve in the region $0 \le h \le h_f$ has been obtained in [26]:

$$\lim_{N\to\infty} \mathcal{C}_R^{Sym} = 1 - \sqrt{\frac{1-\gamma}{1-h^2}} \, . \qquad (11)$$

For finite N, we clearly see a deviation of the concurrence calculated with a state which violates the $\mathbb{Z}_2$ spin-flip invariance from the concurrence evaluated with a state which conserves the latter symmetry. This is indeed a finite-size effect which is beyond the scope of the first order quantum corrections performed in Ref. [26]. In fact, the difference between $\mathcal{C}^{Sym}$ and $\mathcal{C}^{Broken}$ is of order $1/N^2$ as shown in the inset of Fig. 1 [31].

XY model The transverse XY model is defined by the Hamiltonian [23]

$$H_{XY} = -\frac{1}{4}\sum_i \left(\sigma_x^i\sigma_x^{i+1} + \gamma\,\sigma_y^i\sigma_y^{i+1}\right) - h\sum_i \sigma_z^i, \qquad (12)$$

where h is the transverse field strength and γ the anisotropy parameter. Below the quantum critical field $h_c = (1+\gamma)/4$ the parity symmetry is broken; the factorizing field is at $h_f = \sqrt{\gamma}/2$. We numerically computed the ground state nearest neighbor (n.n.) concurrence by means of the Density Matrix Renormalization Group [29]. This powerful numerical technique finds an optimal truncated bases of size $m \sim 100 - 200 \ll 2^N$ to describe the spin chain wave function keeping the desired precision [30]. In Fig. 2 we show the results of the numerical simulations for the concurrence of the central spins (in order to minimize boundary effects) of a chain of length $N = 199$ and different anisotropy values. The concurrence for the even sector $\mathcal{C}^{Sym}$ and broken symmetry ground state $\mathcal{C}^{Broken}$ are then compared for different anisotropy values. The concurrence vanishes at the factorizing field and its derivative with respect to the transverse field at the critical point diverges as expected [1]. The even and odd sector concurrences are found to coincide for the parameter range we considered (data not shown). We used an additional field h_B along σ_x to break the symmetry; our results are stable with respect to changes in the field strength $h_B \in [10^{-4} : 10^{-8}]$ and the field direction in the XY plane (data not shown). Below the factorizing field the concurrence of the broken symmetry and even ground state are clearly different while they are equal between the factorizing and the critical field as there the condition (5) holds [25]. In

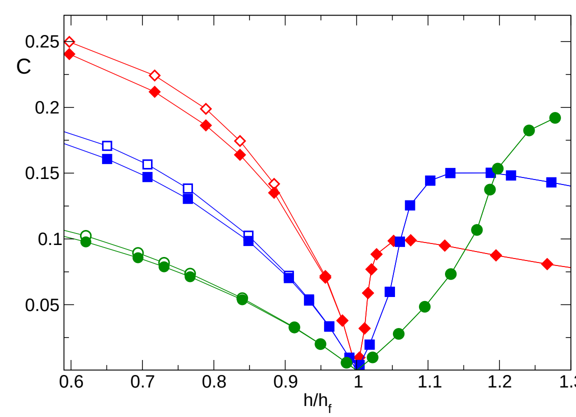

FIG. 2: N.n. concurrence for the anisotropic XY model for $N = 199$, $\gamma = 0.3, 0.5, 0.7$ (circles, squares and diamonds respectively), $m = 200$ in the even sector (full) and for the state with $h_B = 10^{-6}$ (empty).

Fig. 3 we plot the difference between the broken symmetry concurrence and the concurrence in the even sector from the data of Fig. 2. As expected, for $h/h_f \ge 1$ the difference is zero while on the left of the factorizing field

$(h/h_f < 1)$ the difference is not negligible. The inset of Fig. 3 reports the finite size scaling of $|\mathcal{C}^{Sym}$ - $\mathcal{C}^{Broken}|$. Differently from the LMG Model, the broken symmetry effect on the concurrence does not vanish in the thermodynamic limit. It approaches a non-zero value with oscillating behavior. This means that for the XY model conditions (7)-(9) and thus Eq. (5) are violated below h_f.

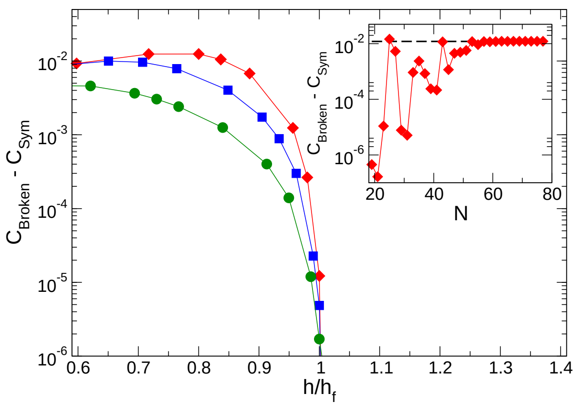

FIG. 3: Difference of the n.n. concurrence in the even sector and for the symmetry broken ground state from the data of Fig. 2 as a function of the transverse field. The maximum relative deviation amounts to around 10%, decreasing with γ for sufficiently small h. Inset: Finite size scaling for $\gamma = 0.7$ and $h/h_f = 0.8$ (diamonds) and limiting value (dashed line).

<u>Conclusions</u> We have found conditions on spin correlation functions, which ensure that the concurrence is invariant respect to breaking of a parity symmetry. They are necessary and sufficient in a regime complementary to where the relations from Ref. [21] do apply. For mean field exact models, one of the conditions (Eq. 7) is satisfied and hence will the rescaled concurrence be unaffected by parity symmetry breaking. The further conditions (Eqs. 8, 9) only emerged for the reduced two-site density matrix having rank three or less. Interestingly, this occurs for the whole system being in a W-type state with two running flipped spins in the ferromagnetically polarized state and a W or GHZ-state, respectively. It would be interesting to verify, whether such states may satisfy the corresponding condition on correlation functions; W-states would lead to a long range concurrence, which has been observed in [13] close to the factorizing point. Numerical studies reveal that the concurrence is affected by symmetry breaking for the LMG and the XY model. As a consequence, the conditions (7)-(9) on the spin correlations are violated up to perhaps a single value for the magnetic field in the LMG model. We gave certain conditions that might admit scenarii different from a robust concurrence between h_c and h_f. Their investigation could provide important insight in the interplay of entanglement and quantum phase transitions.

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[31] an analytical proof of this assumption is left to a future publication.