Four-concurrence in the transverse $XY$ spin-1/2 chain

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(Received 8 June 2017; published 26 July 2017)

We analyze the entanglement measure $C_4$ for specific mixed states in general and for the ground state of the transverse $XY$ spin-1/2 chain. We find that its factorizing property for pure states does not easily extend to mixed states. For cases where the density matrix is a tensor product, $C_4$ is definitely upper bounded by the product of the corresponding concurrences. In transverse $XY$ chains, we find that for large distances this condition goes conform with the working hypotheses of a factorizing property of density matrices in this limit. Additionally, we find that $C_1$ together with the genuine multipartite negativity makes it impossible to decide—at the present state of knowledge—which type of entanglement prevails in the system. In particular, this is true for all entanglement measures that detect SL-invariant genuine $n$-partite entanglement for different $n$. Further measures of SL-invariant genuine multipartite entanglement have to be considered here. $C_4$ is, however, of the same order of magnitude as the genuine multipartite negativity in Phys. Rev. B 89, 134101 (2014) and shows the same functional behavior, which we read as a hint towards the Greenberger-Horne-Zeilinger (GHZ) type of entanglement. Furthermore, we observe an interesting feature in the $C_4$ values that resembles a destructive interference with the underlying concurrence.

DOI: 10.1103/PhysRevA.96.012331

I. INTRODUCTION

Entanglement is a resource in physics and therefore needs to be quantified and to be better understood. For this purpose, it is of major importance to quantify and classify entanglement in laboratory systems, hence for mixed states. In the year 2002, the works [1,2] have initiated an avalanche of analysis into this direction in the following decade. Particular importance was drawn to the Coffman-Kundu-Wootters (CKW) inequality [3], which connected the total entanglement detectable—the tangle: a quantity that originates in the single site reduced density matrix—with something not encoded in the entanglement of pairs, as measured by the concurrence. The difference of the tangle and the sum of the concurrences squared was henceforth interpreted as residual entanglement. The residual entanglement vanishes for the $W$ states and is maximal for any maximally entangled state with respect to the group $SL(2)$ [4–6]. The CKW conjecture could be proved in 2006 by Osborne and Verstraete in Ref. [7]. As a matter of fact, the residual tangle was shown to be dominant not only for the transverse $XY$ model [8]. This means that most of the present quantum correlations close to its quantum phase transitions must come from genuine multipartite entanglement in the spirit of Ref. [4]. Since then, there have been only few recent trials of looking into that direction [9,10]. Here, we will follow this road with an entanglement measure, which is the four-concurrence $C_4$, the four-particle generalization of the concurrence $C_2$. It has been introduced for pure states in Ref. [11] and its convex roof extension is due to Uhlmann [12]. This choice is rather obviously taken with regard to its simple handling and in that it only detects states of Greenberger-Horne-Zeilinger (GHZ) type together with products of two-site entangled states as the Bell states [13]. So besides a possible bipartite part, any further entanglement detected by it will be of GHZ type.

The genuine multipartite negativity [14] is detecting states that are not biseparable. Therefore it will not detect products of Bell states, but it will detect states of W type. Now, when looking at $C_4$ in parallel to the genuine multipartite negativity only, we cannot certify GHZ-type entanglement either, as an outcome of this work, since the negativity may only detect entanglement of W kind, and $C_4$ detects also mixtures of $W$ states and biseparable products of Bell states. The results will therefore be at most a hint towards GHZ entanglement in this model.

This work is laid out as follows: we begin with a study of $C_4$ for specific mixed states in the following section. Next, we analyze this quantity for the transverse Ising model followed by the $XY$ model. The conclusions are drawn and an outlook on possible future directions is given in the last section.

II. THE ENTANGLEMENT MEASURE $C_4$

We highlight on an SL invariant measure of entanglement, the four-concurrence $C_4[\psi] := |\langle \psi^* | \sigma_2^x | \psi \rangle|$ in this work. Whereas this measure cannot distinguish between entanglement that is carried by the states like $|GHZ_4\rangle = \frac{1}{\sqrt{2}}(|0000\rangle + |1111\rangle)$ from that carried by products of Bell states, it will not detect any entanglement supported by states of W type [4,5,13]. The only SL-invariant entanglement measure that detects these globally entangled states (but not genuinely multipartite entangled states, following the notion in Ref. [5]) is the concurrence for two qubits [15,16]. Therefore, in our notion, the W states are only pairwise entangled but which is globally distributed. The convex-roof extension of $C_4$ is calculated for mixed states in the following way [12]:

\begin{align*}
\Sigma_4 & := \sigma_y \otimes \sigma_y \otimes \sigma_y \otimes \sigma_y, \\
R & := \sqrt{\rho} \Sigma_4 \rho^* \Sigma_4 \sqrt{\rho}, \\
C_4[\rho] & = 2\lambda_{\text{max}} - \text{tr} \sqrt{R},
\end{align*}
where $\lambda_{\text{max}}$ is the maximal eigenvalue of the non-negative operator $\sqrt{R}$. At first, we briefly analyze the four-concurrence for certain mixed states.

Since the four-concurrence of a tensor product of Bell states is also maximal as for GHZ states, we have two different classes of entanglement, which do interfere—genuinely entangled GHZ states and biseparable products of Bell states. Hence it is not surprising that for the state $\rho(p) = p|\text{GHZ}_4\rangle\langle \text{GHZ}_4| + (1-p)|\text{Bell} \otimes \text{Bell}\rangle \langle \text{Bell} \otimes \text{Bell}|$, with $|\psi_B \otimes \phi_B\rangle = (|\sigma\sigma\rangle + |\bar{\sigma}\bar{\sigma}\rangle) / \sqrt{2}$ and $|\sigma\bar{\sigma}\rangle = 0$, both entanglement classes interfere such that $C_{4}[\rho(1/2)]$ assumes its minimal value at zero if the states are orthogonal to each other and it can take decreasing values from at most $1/\sqrt{2}$ down to 0 if $|\psi_B \otimes \phi_B\rangle$ is nonorthogonal to GHZ$_4$ (see Fig. 1). This does not happen to be the case for admixtures of a W$_4$ state, it does not lead to an interfering behavior as in the case of three qubits [17]; $C_4$ linearly grows in $p$ for $\rho(p) = p|\text{GHZ}_4\rangle\langle \text{GHZ}_4| + (1-p)|\text{W}_4\rangle \langle \text{W}_4|$, or $\rho(p) = p|\Phi^+ \otimes \Phi^+\rangle \langle \Phi^+ \otimes \Phi^+| + (1-p)|\text{W}_4\rangle \langle \text{W}_4|$ from 0 to 1. Here, we use the standard notation for Bell states: $|\Phi^\pm\rangle = (|11\rangle \pm |00\rangle) / \sqrt{2}$ and $|\psi^\pm\rangle = (|10\rangle \pm |01\rangle) / \sqrt{2}$. In contrast, it will, of course, influence the concurrence when tracing out arbitrary two qubits, as is shown in Fig. 2. Here, we even have a whole interval where $C_4$ is positive and the corresponding concurrences vanish. This behavior changes whenever the state is a tensor product of two two-site matrices; then the optimal decomposition for the concurrences becomes a decomposition of $C_4$, and therefore $C_4$ is upper bounded by the product of the concurrences. An example is shown in Fig. 3 where we plotted $C_4$ of $\rho_4$ together with the products of the corresponding concurrences $C_3$ of the corresponding states $\rho_2$. The density matrix is $\rho_4 = \rho_2 \otimes \rho_2$ with the two-site density matrix $\rho_2 = p|\text{Bell}_1\rangle \langle \text{Bell}_1| + (1-p)|\text{Bell}_2\rangle \langle \text{Bell}_2|$, where $|\text{Bell}_i\rangle$ is an arbitrary Bell state for $i = 1, 2$.

We want to emphasize here that one can not infer from a relation of $C_4$ to the corresponding concurrences anything about the entanglement type participating in the state at hand. For tensor products of density matrices, the factorizing property of $C_4$ is relaxed in that here $C_4$ is upper bounded by the product of the corresponding concurrences.

We now discuss rank-three states. There are several interesting cases for the admixtures of GHZ$_4$ states, products of Bell states, and W$_4$ states. For GHZ$_4 - \text{Bell} \otimes \text{Bell} - \text{W}_4$, mixtures and products of GHZ$_4$ and two different products of Bell states, there can appear whole regions where $C_4$ is zero (see Figs. 4 and 5). However, it is unclear to assign which of the two classes contributed mainly to the state. This becomes particularly clear when no genuinely multipartite entangled state is in the optimal decomposition as it is shown in Figs. 6 and 7. Also in this case, as for rank-two density matrices, a zero in the product of the two concurrences in a particular 2-2 bipartition, which is satisfied for an almost chocklike range, does not mean
The density matrix is taken to be \( \rho \mid W \rangle \rangle \langle W \rangle \) and any biseparable Bell products. Whereas the W state that necessarily \( C_4 = 0 \) (this is only satisfied precisely on the centerline of the two Bell states), as one could erroneously conclude from the fact that \( C_4 \) for pure states decomposes into a product of any two concurrences. The revival for the product of the concurrences from \( q \sim 0.83 \) quadratically to 0.25 at \( q = 1 \) is merely due to the W state (see Fig. 7).

For the mixture of two GHZ states and the W state, we have the same situation as in Fig. 6; the only difference being that the product of the concurrences is always zero except of its quadratic raise from \( q \sim 0.83 \) to 0.25 at \( q = 1 \) as in Fig. 7. We thus cannot learn from \( C_4 \) alone about the nature of entanglement of the state.

With results as those from the PPT criterion [10], we can at best conclude that the state contains entanglement, which is not biseparable in a region where the genuine multipartite negativity \( N_g \) is nonzero [10]. This also includes mixtures of the W state and any biseparable Bell products. Whereas the W state will be detected by the PPT criterion, the products of Bell states would be detectable by \( C_4 \). In order to decide to which class of entanglement a mixed state belongs, we need either a better knowledge of optimal decompositions or different measures of entanglement that do only measure SL-invariant genuine multipartite entanglement [5].

III. THE TRANSVERSE ISING MODEL

Next, we analyze the spin-1/2 Ising model, which is given through the Hamiltonian

\[
H = -\lambda \sum_i S_i^x S_i^y - \sum_j S_j^z.
\]  

(4)

This model has a second-order phase transition from antiferromagnetism at \( \lambda < -1 \) via the paramagnetic phase at \( \lambda \) to ferromagnetism at \( \lambda > 1 \). It is translational invariant and hence we have for the concurrence between sites \( j_1 \) and \( j_2 \) that \( C_2(j_1,j_2) = C_2((j_2-j_1)) = C_2(d) \) for \( d \in \mathbb{Z} \) and \( C_2(-d) = C_2(d) \) with \( C_2(0) := 0 \). Since \( C_2(d) \) vanishes for
an upper bound to decomposition of the optimal decomposition to the concurrences becomes a product of two two-site matrices \[ \text{examples are usually states highlighted here that whenever the state would become a tensor are nearest neighbors with a distance of 1. We want to} \]
\[ \lambda \]
occurs (sometimes called in the literature “sudden death” and of the nearest-neighbor concurrence. Whereas this is not true that the expected result would be upper bounded by the square distances \[ \text{distances} \]
\[ d > 2 \text{, the monogamy relation is easily obtained [8], demonstrating that the essential entanglement in the tansverse Ising model must be of some multipartite type (see Fig. 8). Of what type, however, has never been investigated and even the recent contributions ([9] and [10]) can not distinguish W from GHZ entanglement. Recent discoveries would render this, however, a feasible task [18,19].}

We analyze the entanglement measure \( C_4 \) for this model and compare with the results from Ref. [10]. Therefore we briefly introduce our notation: we write \( C_4(n_1, n_2, n_3) \), where the numbers \( n_i \) indicate how far away to the right is the next neighbor. \( C_4(1,1,1) \) hence means that all neighbors are nearest neighbors with a distance of 1. We want to highlight here that whenever the state would become a tensor product of two two-site matrices [examples are usually states with distances \( (i,n,j) \) when \( n \to \infty \), then, as stated before, the optimal decomposition to the concurrences becomes a decomposition of \( C_4 \), and therefore \( C_4 \) is upper bounded by the product of the concurrences. Therefore we compare the curves for \( C_4(i,n,j) \) with take the product of the two major entanglements \( C_2(i)C_2(j) \). This means that we compare \( C_2^2(1) \) with \( C_4(1,n,1) \), and \( C_2(1)C_2(2) \) with \( C_4(1,n,2) \).

We start our discussion with \( C_4(1,n,1) \). Observing that the nearest-neighbor concurrence is nonzero and assuming that the density matrix be a tensor product for \( n \to \infty \), we deduce that the expected result would be upper bounded by the square of the nearest-neighbor concurrence. Whereas this is not true for \( n = 2,3 \) it begins to be satisfied for growing \( n \), where a gap occurs (sometimes called in the literature “sudden death” and “sudden revival” of entanglement) around the critical point \( \lambda_c = 1 \) (see Fig. 9). Since the state should become a tensor product only for \( n \to \infty \), the results are not violating this working hypothesis of earlier work. That it is not satisfied for \( n = 2,3 \) is not so surprising, \( C_4 \) being zero means that the density matrix can be decomposed in this region into states exclusively from the null cone of \( C_4 \), that means none of the states is of the GHZ type or a tensor product of Bell-like states in whatsoever bipartitions of the four-site subsystem. This does not mean, however, that the decomposition could not be genuinely multipartite entangled, since it includes, e.g., the genuinely four-partite entangled Cluster states and \( X \)-type states, as seen in Fig. 6. In addition, the optimal decompositions for \( C_4 \) and the genuine multipartite negativity could be different, a phenomenon that occurred, e.g., in Ref. [17], and created some ambiguity in the types of entanglement that may enter a decomposition. We want to mention here that for configurations \( (1,n,1) \) and \( n \geq 3 \) the genuine multipartite negativity is zero. Hence the entanglement has its origin in biseparable products of Bell states there. We highlight that our results go conform with the genuine multipartite negativity being zero for these instances.

The same argument would apply to \( C_4(2,n,2) \) and \( C_4(1,n,2) \) or equivalently \( C_4(2,n,1) \), but in these cases \( C_4 \) always turns out to be zero, except for \( C_4(1,1,2) \), which we show in Fig. 10. It is important to mention here that \( C_4(2,n,2) \) being zero does not violate the working hypothesis that this state roughly becomes a tensor product with growing \( n \), either. Here, the states in the optimal decomposition are in the null cone of \( C_4 \) for all \( C_4(2,n,2) \), and for \( n > 2 \) in \( C_4(1,n,2) \), whereas there is still a possibility for the GHZ state left to support the entanglement as long as \( C_4 \) is zero (see, for instance, finite regions with \( C_4 = 0 \) in Figs. 4 and 5).
shown together with $C_4(1, n, 2)$ that exists.

## IV. THE TRANSVERSE XY MODEL

The Hamiltonian is

$$H = -\lambda \sum_i \left( \frac{1 + \gamma}{2} S_i^x S_i^x + \frac{1 - \gamma}{2} S_i^y S_i^y \right) - \sum_i S_i^z$$

and, except for $\gamma = 0$, the model is in the same universality class with the transverse Ising model. When going towards the isotropic model at $\gamma = 0$, the range $R$ of the concurrence $C_2(n)$ grows as $R \propto \gamma^{-1}$ for the critical value $\lambda_c$ (see Ref. [20]). The model hence interlinks the Ising case for the anisotropy parameter $\gamma = 1$ with the isotropic model for $\gamma = 0$. It has a factorizing point $\lambda_f = (1 - \gamma^2)^{-1/2}$. Here, the ground state of the chain is compatible with the necessary condition that $C_4(1, n, 1)$ be smaller than $C_2(1)^2$ for $\lambda \geq \lambda_f$ and $n \geq 4$; for $\lambda \leq \lambda_f$ this condition is violated. For $n \geq 5$ and $\lambda \leq 1.125$, it is satisfied again (see inset of Fig. 11). $C_4(2, n, 2)$ is considerably large for sufficiently small $n$ only. Therefore we print it only for the values $n = 1, 2$ in Fig. 12 and compare it against the concurrence squared $C_2(1)^2$. That $C_4(2, n, 2)$ is larger than $C_2(1)^2$ in a wide region for $n = 1, 2$ just tells that the state has not a product form here, hence it could be otherwise entangled; for higher values of $n$.
and the state satisfies the condition for being (roughly) a product in these cases.

Next, we look at 1-1-n configurations. This state should become a tensor product for growing number of n. Hence its four-concurrence should tend to zero. We analyze the four-concurrence $C_4(1,1,n)$ for different values of the anisotropy parameter $\gamma$ and for $n = 2$ and 3. We observe that $C_4(1,1,2)$ does not differ much for the values of $\gamma$ from 0.55 via 0.58 to 0.59 (Figs. 13, 15, and 17) beside the shift of the factorizing point following $\lambda_f = (1 - \gamma^2)^{-1/2}$. The interval of $\gamma$ is chosen such that $C_2(3)$, at the critical value, drops to zero a bit before $\gamma = 0.58$. Something interesting begins to happen, when the four-concurrence of the distance 1-1-3 is considered. Whereas for $\gamma = 0.55$, $C_4(1,1,3)$ sets in considerably before $C_2(1)C_2(3)$ begins to have nonvanishing values from about $\lambda = 0.975$, with a visible finite slope, a bit before the critical point $\lambda_c$ (see Fig. 14). Then, $C_2(1)C_2(3)$ behaves as if it were “pinned” at the critical point $\lambda_c$ for the following two values of $\gamma = 0.58$ (both curves with a rather high slope; see Fig. 16) and $\gamma = 0.59$ (again with a visible slope; see Fig. 18).

$C_4(1,1,3)$ is definitely feeling the critical point as well: whereas its onsetting remains at about the same distance from the point where $C_2(1)C_2(3)$ sets in from $\gamma = 0.55$ to $\gamma = 0.58$ it, however, squeezes the function $C_2(1)C_2(3)$ against the critical point, and thereby also feels an apparently destructively interfering part from it [see the maximum of $C_4(1,1,3)$ in Fig. 16]. At $\gamma = 0.59$, $C_4(1,1,3)$ has already overtaken $C_2(1)C_2(2)$, the latter being still stuck to the critical $\lambda_c$ but with a visible slope. We remember that a nonvanishing $C_4$ in presence of a zero $C_2(1)C_2(2)$ does not need to mean a nonzero portion of GHZ-like entanglement in principle (see the discussion of Fig. 6), it is, however, an interesting observation.

We have to mention that the function $C_2(3)$, as every entanglement measure, is pinned at and also localized about the factorizing field. Therefore it vanishes for the Ising model [1]. It exists for an arbitrary value of $0 < \gamma < 1$ and will be accompanied by $C_4(1,1,3)$ (also pinned at the factorizing field), getting smaller and smaller as $\gamma \to 1$. Similar conclusions apply also to $C_2(n)$ and we conjecture also the corresponding behavior for $\gamma \to 1$ of $C_4(1,1,n)$, which we leave to possible future publications.
FOUR-CONCURRENCE IN THE TRANSVERSE XY SPIN- . . .

V. CONCLUSIONS AND OUTLOOK

We have analyzed the four-concurrence $C_4$ with particular emphasis on spin-1/2 chains. Similarly to the well known concurrence $C_2$, this measure is an entanglement monotone [23], which has an exact analytic form for arbitrary mixed states, which is due to the fact that it is written as a bilinear form of the pure state coefficients [5,6,12]. Note that this is a nontrivial property since in general one has to minimize over arbitrary decompositions of a given density matrix (convex-roof construction). For example, for the three-tangle [3], the convex roof is unknown for general mixed states. As a drawback, beyond genuine four-partite GHZ-type entanglement, $C_4$ also detects bipartite entanglement such as the product of Bell states. This has to be taken into account when interpreting the results.

As a first and central result, the obvious factorizing property of $C_4$ for pure states $|\Psi_{1,2,3,4}\rangle = |\Psi_{1,2}\rangle \otimes |\Psi_{3,4}\rangle$,

$$C_4(\Psi_{1,2,3,4}) = C_2(\Psi_{1,2})C_2(\Psi_{3,4}),$$

(6)
do not apply to mixed states—instead, we find the inequality for tensor products as $\rho_{1,2,3,4} = \rho_{1,2} \otimes \rho_{3,4}$ (see Fig. 3),

$$C_4(\rho_{1,2,3,4}) \leq C_2(\rho_{1,2})C_2(\rho_{3,4}).$$

(7)

Naively, one might be tempted to interpret the difference between $C_4$ and the product of the concurrences $C_2$ as an indicator for four-partite GHZ-type entanglement. However, this is not correct in general. First, the contributions to $C_4$ stemming from four-partite and pairwise entanglement are not additive, i.e., there can be interferences (see Fig. 1). Second, even if the product of the concurrences $C_2$ vanishes, a nonzero $C_4$ does not necessarily indicate four-partite GHZ-type entanglement (see Fig. 2). This indicates that the optimal decomposition (in the convex roof construction) for $C_4$ is different from that for the two $C_2$. We emphasise that one can apply Eq. (7) to spin models in order to test when a state can roughly be given by a corresponding tensor product.

Next, we evaluate the four-concurrence for the Ising model. We find that $C_4$ for the four nearest neighbors significantly exceeds the product of the concurrences (see Fig. 9), indicating that a product ansatz $\rho_{1,2,3,4} = \rho_{1,2} \otimes \rho_{3,4}$ is not a good approximation here. As suggested by Eq. (7), this approximation should become better when we increase the distance between the two pairs of spins (see Fig. 9). For $n = 1,2$, the four-concurrence $C_4(1,n,1)$ violates the bound (7).

At the critical point, $C_4(1,n,1)$ vanishes for $n \geq 7$; it stays exactly zero in an interval around the critical point (we did not check this for $n > 12$ but formulate it as a surmise here). For configurations of distances 1-7-2, only the case $n = 1$, i.e., $C_4(1,1,2)$ (or equivalently $C_4(2,1,1)$) yields a nonzero result. For $C_4(1,1,2)$ (three neighboring spins while the fourth spin is the next-to-nearest neighbor), we also find a violation of the bound (7); therefore the state is not a simple tensor product. $C_4(2,n,2)$ vanish for all $n$. For the states with distances $(i,n,j)$ and $n \to \infty$, one is roughly left with a tensor product of density matrices and there the four-concurrence $C_4$ must be upper bounded by the product of the concurrences $C_2(i)C_2(j)$. Also here, only a hint towards GHZ-type entanglement for the distances $(1,2,1)$ and $(1,1,2)$ is given from the results for the corresponding genuine negativity that behaves essentially the same way [10]. However, as explained above, additional entanglement measures are mandatory in order to get a clear answer. This holds for any two measures that detect an, e.g., SL-invariant genuine $n$-partite entanglement one wishes to assure in common together with at least one further type of entanglement each in which they differ.

For the XY model, we obtain analogous results below the critical point $\lambda \leq 1$, $C_4(1,n,1)$ is upper bounded by the concurrence $C_2(1)^2$ for $\lambda \geq 0$ and $\lambda \leq 1.025$ vanishes precisely for $n \geq 7$ close to the critical point. One noticeable difference to the Ising model is the factorizing (Kurmann-Thomas-Müller) point [21]. At this factorizing point, this is not the case. We obtain different behavior for $\lambda \in [\lambda_c, \lambda_f]$ and $\lambda > \lambda_f$: between the critical point (at $\lambda_c = 1$) and this factorizing point ($\lambda_f = 2/\sqrt{3}$ for $\gamma = 1/2$), the four-concurrence $C_4(1,n,1)$ violates the bound (7) for $n < 5$ in $\lambda \in [\lambda_c,1.125]$ and close to the factorizing point for $n$ smaller than 7 or 8; above this factorizing point, the bound is violated for $n < 4$ (see Fig. 11).

Additionally, we find a nonzero $C_4(2,1,2)$ (see Fig. 12) that, however, violates Eq. (7). Analyzing $C_4(1,1,1)$ for $n = 2,3$, we observe a further unexpected phenomenon. Particularly interesting is the functional dependence of $C_4(1,1,3)$ on the parameter $\lambda$. It is rather complex and changes drastically when going from $\gamma = 0.58$ to $\gamma = 0.59$. This suggests interference effects, which needs further analysis.

Note added. Recently, there has been significant progress in estimating tangles in general [24,25] and for the XY model in particular [26].

ACKNOWLEDGMENTS

We acknowledge financial support by the German Research Foundation within the SFB TR12 and SFB 1242.