Finite size effects in entangled rings of qubits

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We study translationally invariant rings of qubits with a finite number of sites \( N \), and find the maximal nearest-neighbor entanglement for a fixed \( z \) component of the total spin. For small numbers of sites our results are analytical. The use of a linearized version of the concurrence allows us to relate the maximal concurrence to the ground state energy of an XXZ spin model, and to calculate it numerically for \( N \leq 24 \). We point out some interesting finite-size effects. Finally, we generalize our results beyond nearest neighbors.

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I. INTRODUCTION

Entanglement in many-body systems such as spin chains has recently attracted much attention. The reasons are at least twofold: on one side one is interested in understanding fundamental structures of entangled multipartite states and the natural occurrence of such states in systems with spin-spin interactions, with quantum information processing purposes in mind. On the other side insights from quantum information theory may lead to a deeper understanding of many-body phenomena in strongly interacting systems, such as quantum phase transitions and critical behavior.

Much effort has been devoted to studying the natural appearance of bipartite entanglement in ground states of 1-dimensional spin models with an Ising Hamiltonian or a Heisenberg-type Hamiltonian \[1, 2, 3, 4\], with special emphasis on properties of entanglement near a quantum phase transition. It has been pointed out that some entanglement remains for finite temperatures (so-called thermal entanglement \[5\]), which for some transverse field can even increase with increasing temperature. Recently, it has been shown that maximally entangled states of atoms can be created by crossing a quantum phase transition \[6\].

A complementary approach to the phenomenon of entanglement in chains of qubits has been initiated by O’Connor and Wootters \[7\] (see also \[8\]): they ask (without specifying a Hamiltonian) the fundamental question “what is the maximal entanglement between two neighboring sites of an entangled ring with translational invariance”? An “entangled ring” is defined as a chain of qubits with periodic boundary conditions. Due to the so-called “monogamy of entanglement” it is impossible for a site to be maximally entangled with both its neighbors: shared entanglement is always less than maximal \[9, 10\]. In Ref. \[7\] the question of the upper limit for the nearest neighbor entanglement was simplified by introducing two additional restrictions on the allowed states:

(i) the state is an eigenstate of the \( z \) component of the total spin,
(ii) neighboring spins cannot both be “up”.

Both restrictions are based on an educated guess for the optimal states for the general problem. O’Connor and Wootters solved the restricted optimization problem by relating it to an effective Hamiltonian for the one-dimensional ferromagnetic \( XY \) model, and found the maximal nearest-neighbor concurrence to be

\[
C_{\text{max}}(N, p) = \frac{2 \sin \left( \frac{p \pi}{N} \right)}{N \sin \left( \frac{\pi}{N} \right)},
\]  

where \( N \) is the number of sites and \( p \) is the number of up-spins. Eq. \[1\] provides a lower bound for the problem without restriction (ii). For given \( N \) and \( p \), it may or may not happen that \( C \) can be increased by also allowing states where two neighboring spins are up. In the limit \( N \to \infty \), the optimal number of up-spins in Eq. \[1\] approaches \( p_{\text{opt}} \approx 0.301 N \). This leads to an asymptotic value of \( C_{\text{max}} \approx 0.434 \). Whether this number can be improved by removing restriction (ii) or restriction (i) is an open problem. We will illustrate, however, that for a fixed \( p \) restriction (ii) tends to play a decreasing role as \( N \) is increased.

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In this article we mainly focus on the problem of optimizing the nearest-neighbor entanglement for given finite \( N \) and \( p \), without imposing restriction (ii). Using the methods described below we solve a number of cases analytically. We supplement these results by numerical calculations, and thus arrive at a rather complete picture of the solutions for \( N \leq 24 \). Some finite size effects that occur only for specific small numbers of sites will be pointed out.

The paper is organized as follows: In Sec. I we introduce the problem and our notation, and study symmetry under reflections. In Sec. II we describe our analytical results for the maximal nearest-neighbor entanglement in the cases \( p = 2 \) and \( p = N/2 \). In Sec. III we numerically investigate whether the solutions in II are at least still local maxima when restriction (ii) is removed. In Sec. IV we use a method recently introduced by Wolf et al. [11], mapping the original nonlinear problem onto a series of linear ones. We discuss some general properties of the mapping, and use it to numerically calculate the maximal nearest-neighbor concurrence for \( N \leq 24 \). Finally, in Sec. VII we discuss our results and point out some interesting questions that are still open.

II. MAXIMAL NEAREST NEIGHBOR ENTANGLEMENT

We consider a ring of \( N \) qubits, out of which \( p \) are in the state \( |↑⟩ \) and \( N−p \) are in the state \( |↓⟩ \). In the following we will use the notation \( |↓⟩ = |0⟩ \) and \( |↑⟩ = |1⟩ \), and will refer to \( p \) as the occupation number. We will always consider translationally invariant states.

A. Translationally invariant states and concurrence

Our aim is to calculate the maximal nearest-neighbor entanglement of two qubits, using the concurrence as a measure. The concurrence is defined as [12] \( C(\rho) = \max\{\lambda_1 - \lambda_2 - \lambda_3 - \lambda_4, 0\} \), where \( \lambda_1 \geq \lambda_2 \geq \lambda_3 \geq \lambda_4 \geq 0 \) are the square roots of the eigenvalues of \( \rho \tilde{T} \), and \( \tilde{T} := (\sigma^y \otimes \sigma^y)\rho(\sigma^y \otimes \sigma^y) \) is the spin-flipped density matrix.

The structure of any two-qubit reduced density matrix on the ring is, due to the properties of translational invariance, substantially simplified by requiring \( v = 0 \), i.e. two neighboring spins cannot be both “up”. This is the assumption that was made in II — we will relax this constraint throughout our work.

For given \( N \) and \( p \) we apparently need to maximize Eq. (3) over all translationally invariant states, that is, over all density matrices fulfilling \(|\varrho, \varpi⟩⟩ = 0 \), where \( \varpi \) is the operator that implements a translation by one site. As was shown in II, the problem splits into \( N \) maximization problems over pure states: since \( \varrho \) and \( \varpi \) commute, the spectral decomposition of \( \varrho \) can be expressed in projectors onto eigenstates of \( \varpi \), namely

\[
\varrho = \sum_{k=0}^{N-1} p_k |\psi_k⟩⟨\psi_k|,
\]

where \( p_k \geq 0 \) and \( \sum_k p_k = 1 \). Here the eigenstates of the translation operator are defined by \( \varpi |\psi_k⟩ = e^{i\frac{2\pi k}{N}} |\psi_k⟩ \).

Since \( C \) is a convex function, we have

\[
C\left(\sum_k p_k |\psi_k⟩⟨\psi_k|\right) \leq \sum_k p_k C(|\psi_k⟩⟨\psi_k|) \leq \max_k \{C(|\psi_k⟩⟨\psi_k|)\},
\]
and it is thus sufficient to first maximize the concurrence over pure states within each eigenspace of the translation operator, and then choose the maximal result over all eigenstates. In fact, the situation is even simpler, since, as shown in [3], the search can be restricted to the $k = 0$ eigenstates, i.e. to eigenstates of $T$ with eigenvalue 1.

For a given number of sites $N$ and a given occupation number $p$, the most general eigenstate of $T$ with eigenvalue 1 is a superposition that looks as follows:

$$|\psi(N, p)\rangle = \sum_\mu a_\mu |\mu\rangle,$$

with the normalizations

$$\langle \mu | \mu \rangle = 1 \quad \text{and} \quad \sum_\mu |a_\mu|^2 = 1,$$

and with

$$|\mu\rangle = N_\mu \sum_{j=0}^{N-1} T^j |\phi_\mu\rangle.$$

The above notation is as follows: the index $\mu$ enumerates all distinct translationally invariant configurations of the ring where the $p$ up-spins and $(N - p)$ down-spins have given relative positions. The state $|\phi_\mu\rangle$ is one representative member of the $\mu$th configuration. The operator inducing a translation by $j$ sites is given by $T^j$, and $N_\mu$ denotes an appropriate normalization factor. Thus, $|\mu\rangle$ is a normalized eigenstate of $T$ corresponding to the configuration $\mu$ and the eigenvalue 1. Note that for a given $\mu$ it may happen that $T^j |\phi_\mu\rangle = |\phi_\mu\rangle$ already for $j = \tilde{N} < N$; in that case it is not possible to construct eigenstates corresponding to all eigenvalues of $T$ from $|\phi_\mu\rangle$. This is accounted for by an appropriate value of $N_\mu$, which in the general case $(\tilde{N} \leq N)$ reads $N_\mu = \sqrt{N/\tilde{N}}$.

We use the following convention to denote $\mu$ explicitly: the composite index $\mu$ consists of $p$ entries, where each entry specifies a distance from one up-spin to the next up-spin in $|\phi_\mu\rangle$. We choose the first entry to be the smallest. Note that the $p$ entries add up to $N$. An example will clarify this notation: let us consider the case of $N = 5$ qubits and the occupation number $p = 2$. Then the index $\mu$ can only take two combinations of entries, namely 1,4 and 2,3. The most general translationally invariant state with translational eigenvalue 1 is written as

$$|\psi(N = 5, p = 2)\rangle = a_{1,4}|1, 4\rangle + a_{2,3}|2, 3\rangle$$

$$= \sum_{\mu = 1, 4, 2, 3} a_\mu \frac{1}{\sqrt{5}} \sum_{j=0}^{4} T^j |\phi_\mu\rangle$$

$$= a_{1,4} \frac{1}{\sqrt{5}}(|11000\rangle + |01100\rangle + |00110\rangle + |00011\rangle + |10001\rangle) +$$

$$a_{2,3} \frac{1}{\sqrt{5}}(|10100\rangle + |01010\rangle + |00101\rangle + |10010\rangle + |01001\rangle),$$

where the normalization reads $|a_{1,4}|^2 + |a_{2,3}|^2 = 1$. The task is then to find the optimal coefficients $a_\mu$, such that $C$ is maximized.

**B. Reflection symmetry**

One main big difficulty in the maximization problem of the concurrence is the growing number of free parameters $a_\mu$ for higher $N$ and $p$ [10]. In this subsection we will elaborate on a symmetry argument that eliminates nearly half of the parameters.

Recall the state under consideration, Eq. (6), and the definition of the $p$-dimensional index $\mu$, which specifies the number of steps from one up-spin to the next. It is clear that a cyclic permutation of the entries of $\mu$ will always result in the same state $|\mu\rangle$, whereas an anti-cyclic one will result in a state where all spins are reflected around a certain site. Since $|\mu\rangle$ is translationally invariant, it does not matter around which site the reflection is performed, and for convenience we can assume that the reflection interchanges the two sites that we are focusing on. Denoting the reflection operator by $R$, it is then obvious that $\varrho \rightarrow R\varrho R$ leads to $\varrho^{(2)} \rightarrow [\varrho^{(2)}]^T$ (in our chosen basis) for any translationally invariant $\varrho$. In terms of the matrix elements, reflection causes $v, w, y \rightarrow v, w, y$ while $z \rightarrow z^*$. In particular the reflected state has the same concurrence as the original one, $C(R\varrho R) = C(\varrho)$.
Now, let us study the entanglement properties of $\tilde{\rho} = (\rho + R \rho R) / 2$. We arrive at

$$C(\tilde{\rho}) = |z + z^*| - 2 \sqrt{\frac{1}{2} (v + v) \frac{1}{2} (y + y)} = C(\rho),$$

and thus it is sufficient to consider states of the form $\tilde{\rho}$. Note that $\tilde{\rho}$ commutes with the reflection operator, i.e. $[\tilde{\rho}, R] = 0$, and therefore can be decomposed into projectors onto eigenstates of the reflection operator. By the same argument that allowed us to reduce the original problem to a pure state problem for each translational eigenvalue, we can now restrict our attention to pure states with translational eigenvalue $1$ and odd or even reflection symmetry. In fact, using the observation from [7] that one only needs to consider positive coefficients $a_\mu$ in the optimal state, we immediately find that the even states will contain an optimal state. This result is non-trivial, intuitive as it may seem: A non-linear optimization problem could lead to solutions that break the underlying symmetries. Here, however, this is not the case and this fact reduces the dimensionality of the relevant parameter space significantly.

### III. ANALYTICAL RESULTS

In the following we will consider various occupation numbers, starting with the trivial case $p = 1$: here the state is completely fixed and reads

$$|\psi(N, p = 1)\rangle = \frac{1}{\sqrt{N}} \sum_{i=0}^{N-1} T^i|\phi_N\rangle,$$

which is a generalized W-state. The concurrence between nearest neighbors (in fact, between any two sites) is given as $C(N, p = 1) = 2/N$.

#### A. Maximal nearest neighbor concurrence for occupation number $p = 2$

The case $p = 2$ is already much more involved. The concurrence of a given state can still be written in a compact way for all $N$, but it will turn out that the optimization problem can only be solved analytically for some small numbers of sites. The most general translationally invariant state for $N$ sites with occupation number $p = 2$ is given by

$$|\psi(N, p = 2)\rangle = \sum_\mu a_\mu N_\mu \sum_{i=0}^{N-1} T^i|\phi_\mu\rangle,$$

where, as explained above, $\mu$ is a index with two entries which describes the location of the up-spins in the ring: the first value for $\mu$ is $1, N - 1$. As mentioned above, for the optimization problem we can take the coefficients $a_\mu$ to be real and positive.

At this point we have to distinguish the cases of even and odd $N$:

1. **Even $N$**: The index $\mu$ stands for all inequivalent decompositions of $N$ into a sum of two terms, starting at $1, N - 1$, then $2, N - 2$ and so forth until $N/2, N/2$. The last term of the superposition in Eq. (12) is special, because a translation by $N/2$ sites already leads to $T^{N/2}|\phi_{N/2, N/2}\rangle = |\phi_{N/2, N/2}\rangle$. Therefore this contribution has a different normalization, as mentioned below Eq. (12).

This becomes immediately clear from looking at an example; let us choose $N = 4$ and $p = 2$:

$$|\psi(N = 4, p = 2)\rangle = a_{1,3}|1,3\rangle + a_{2,2}|2,2\rangle$$

$$= \sum_{\mu=1,3;2,2} a_\mu N_\mu \sum_{i=0}^{N-1} T^i|\phi_\mu\rangle$$

$$= a_{1,3} \frac{1}{2} (|1100\rangle + |0110\rangle + |0011\rangle + |1001\rangle) + a_{2,2} \frac{1}{\sqrt{2}} (|1010\rangle + |0101\rangle).$$
For better clarity we will from now on simplify the above notation of the composite index µ by dropping the second entry, i.e. $a_{1,N-1} = a_1$ and $|1,N-1\rangle = |1\rangle$ and so forth. (This short-hand notation is of course only possible for the case $p = 2$.) Calculating the matrix elements for even $N$, one finds

\[
y = \frac{1}{N} a_1^2, \tag{14}
\]

\[
v = \begin{cases} 
\frac{1}{N} (N - 4 + a_1^2) & \text{for } N > 3 \\
0 & \text{otherwise}
\end{cases}, \tag{15}
\]

\[
z = \frac{2}{N} \left( \sum_{i=1}^{N/2-1} a_i a_{i+1} + \sqrt{2} a_{N/2-1} a_{N/2} \right). \tag{16}
\]

The concurrence is thus given by the expression

\[
C = \frac{2}{N} \max \left\{ 2|a_1 a_2 + a_2 a_3 + \cdots + a_{N/2-2} a_{N/2-1} + \sqrt{2} a_{N/2-1} a_{N/2}| - |a_1| \sqrt{N - 4 + a_1^2}, 0 \right\}. \tag{17}
\]

(2) Odd $N$:

Here the double index $\mu$ runs from 1, $N - 1$ until $(N - 1)/2, (N + 1)/2$. The normalization of all terms in the superposition is identical. An example of the most general state has already been shown for $N = 5$ in Eq. (9). With the short-hand notation introduced above we find

\[
y = \frac{1}{N} a_1^2, \tag{18}
\]

\[
v = \begin{cases} 
\frac{1}{N} (N - 4 + a_1^2) & \text{for } N > 3 \\
0 & \text{otherwise}
\end{cases}, \tag{19}
\]

\[
z = \frac{2}{N} \left( \sum_{i=1}^{(N-1)/2-1} a_i a_{i+1} + \frac{1}{2} a_{(N-1)/2}^2 \right). \tag{20}
\]

The only differences to the case of even $N$ are the last term in $z$ being $\frac{1}{2} a_{(N-1)/2}^2$ instead of $\sqrt{2} a_{N/2-1} a_{N/2}$, and the upper summation bounds for $z$. The concurrence for odd $N$ reads

\[
C = \frac{2}{N} \max \left\{ 2|a_1 a_2 + a_2 a_3 + \cdots + a_{(N-1)/2-1} a_{(N-1)/2} + \frac{1}{2} a_{(N-1)/2}^2| - |a_1| \sqrt{N - 4 + a_1^2}, 0 \right\}. \tag{21}
\]

From Eqs. (17) and (21) we see immediately that the first amplitude $a_1$ has a special role: it is the only one that appears explicitly in the last term of the concurrence, namely the term $-\sqrt{a_1^2}$. Note that the coefficient $a_1$ specifies the only case where two neighboring spins are up. Considering both terms of the concurrence where $a_1$ appears, we can find a simple argument when the coefficient $a_1$ has to be zero in order to maximize the concurrence: for $N \geq 8$, the inequality

\[
2a_2 - \sqrt{N - 4 + a_1^2} \leq 0 \tag{22}
\]

holds for any $a_2$ and $a_1$. Therefore, the concurrence is always increased by setting $a_1 = 0$. Thus, for more than 8 sites (for both even and odd $N$) and the occupation number $p = 2$ one finds indeed the highest concurrence by using the constraint “no neighboring spins are up”, i.e. $C^{\text{max}}$ is given by Eq. (1). Note, however, that the actual coefficients of the optimal state are not trivial to find from the method in [7]. Thus we have also used an alternative method which employs Lagrange multipliers. Our method does not only provide the value of the maximal concurrence, but also the coefficients $a_\mu$ that define the corresponding state. The details are described in the Appendix. Using this method we find e.g. for the case $N = 8$ and $p = 2$ the results $C^{\text{max}}(N = 8, p = 2) = \sqrt{3}/4$, where the coefficients of the optimally entangled state are given by $a_2 = \sqrt{1/6}, a_3 = \sqrt{1/2}$ and $a_4 = \sqrt{1/3}$.

For $N < 8$ we have in general $a_1 \neq 0$, and the simple method from the Appendix cannot be applied. One has to maximize the concurrence explicitly. This was done for the cases $N = 4$ (here it turns out that one can reach the same concurrence as for $p = 1$, by taking $a_1 = \sqrt{1/3}$ and $a_2 = \sqrt{2/3}$); for $N = 5$ we have only two terms, namely $|N = 5, p = 2\rangle = a_1|1, 4\rangle + a_2|2, 2\rangle$ and arrive at the optimal solution $a_1 = 0.298$ and $a_2 = 0.955$. The case $N = 6$ can
again be solved analytically: if the state is written as $|N = 6, p = 2⟩ = a_1|1, 5⟩ + a_2|2, 4⟩ + a_3|3, 3⟩$, the concurrence reads

$$C(N = 6, p = 2) = \frac{2}{3} \left( \sqrt{1 - a_1^2} - a_3^2 (a_1 + \sqrt{2}a_3) - \frac{1}{2} a_1 \sqrt{2 + a_2^2} \right),$$

where we have eliminated $a_2$ via the normalization constraint. The maximum can be found by demanding that the derivatives with respect to $a_1$ and $a_3$ have to be zero. This leads to the solution $a_1 = 0$ and $a_2 = a_3 = \sqrt{1/2}$ for the maximal concurrence. Finally, for $N = 7$ we have $|N = 7, p = 2⟩ = a_1|1, 6⟩ + a_2|2, 5⟩ + a_3|3, 4⟩$ and

$$C(N = 7, p = 2) = \frac{2}{7} \left( 2a_2 \sqrt{1 - a_1^2 - a_2^2} - (a_1 - a_2)^2 + 1 - a_1 \sqrt{a_2^2 + 3} \right),$$

where this time we have applied the normalization to eliminate $a_3$. Calculating $dC/da_1$, we find that $a_1 > a_2 \Rightarrow dC/da_1 < 0$, whereas $dC/da_2 = 0$ is equivalent to $a_1 - a_2 = (a_2^2 - a_3^2)/a_3$. The last equality can only be fulfilled for (I) $a_1 > a_2 > a_3$, where as noted $dC/da < 0$, for (II) $a_1 = a_2 = a_3$ which is clearly not optimal, or for (III) $a_3 > a_2 > a_1$.

For the last case, we can use again an argument like for $N \geq 8$ to show that $a_1 = 0$, $a_2 = \sqrt{(5 - \sqrt{5})/10}$, and $a_3 = \sqrt{(5 + \sqrt{5})/10}$ is optimal and gives $C_{max}(N = 7, p = 2) = (1 + \sqrt{5})/7$.

This completes the study of the case $p = 2$. To summarize, we have found a simple argument to show the solution in [12] to be optimal for $N \geq 8$ and $p = 2$, and have explicitly performed the optimization for rings with seven or less spins. In the case $N = 5$, the seemingly simple one-parameter optimization results in a fourth-order equation that had to be solved numerically. All other cases were solved analytically. Note that $N = 5$ is the only non-trivial case where the optimal state contains two neighboring up-spins. We summarize the results for occupation number $p = 2$ in Tab. II (see also Fig. II).

| $N$ | $p$ | $C_{max}(N, p)$ | Coefficients |
|-----|-----|----------------|---------------|
| any | 1   | $2/N$          | $a_1 = 1$     |
| 2   | 2   | 0              | $a_1 = 1$     |
| 3   | 2   | $2/3$          | $\approx 0.667$, $a_1 = 1$ |
| 4   | 2   | $1/2$          | $= 0.5$, $a_2 = 1$ |
| 5   | 2   | $\sqrt{2}/3$  | $\approx 0.468$, $a_2 = 0.298$, $a_2 = 0.955$ |
| 6   | 2   | $\sqrt{2}/3$  | $\approx 0.471$, $a_2 = a_3 = \sqrt{1/2}$ |
| 7   | 2   | $(1 + \sqrt{5})/7$ | $\approx 0.462$, $a_2 = \sqrt{2/(5 + \sqrt{5})}$, $a_3 = (1 + \sqrt{5})/\sqrt{2(5 + \sqrt{5})}$ |
| 8   | 2   | $\sqrt{3}/4$  | $\approx 0.433$, $a_2 = 1/\sqrt{6}$, $a_3 = 1/\sqrt{2}$, $a_4 = 1/\sqrt{3}$ |
| 9   | 2   | $4 \cos(\pi/7)/9$ | $\approx 0.400$, $a_2 \approx 0.328$, $a_3 \approx 0.591$, $a_4 \approx 0.737$ |
| 10  | 2   | $\sqrt{2 + \sqrt{2}}/5$ | $\approx 0.370$, $a_2 = (1 - \sqrt{2})/\sqrt{2 + \sqrt{2}}$, $a_3 = 1/2$, $a_4 = \sqrt{(2 + \sqrt{2})/8}$, $a_5 = 1/2$ |
| 11  | 2   | $4 \cos(\pi/9)/11$ | $\approx 0.341$, $a_2 \approx 0.228$, $a_3 \approx 0.429$, $a_4 \approx 0.577$, $a_5 \approx 0.657$ |
| 12  | 2   | $(5 + \sqrt{5})/2/6$ | $\approx 0.317$, $a_2 = \sqrt{2}/(5 + \sqrt{5})$, $a_3 = 1/\sqrt{5 + \sqrt{5}}$, $a_4 = (3 + \sqrt{5})/\sqrt{(2(5 + \sqrt{5}))}$, $a_5 = (1 + \sqrt{5})/(2\sqrt{5} + \sqrt{5})$, $a_6 = (1 + \sqrt{5})/(5 + \sqrt{5})$ |

TABLE I: Maximal nearest-neighbor concurrence and coefficients for the optimal state, with $p = 2$. Only non-vanishing coefficients are given explicitly.

B. Maximal nearest neighbor concurrence for $p = N/2$

The case of half-filling, $p = N/2$, is special because the non-linear form of the concurrence [3] then is reduced to

$$C(N, p = N/2) = 2 \max\{|z| - |v|, 0\},$$

(25)
since here the matrix elements $v$ and $y$ are equal. As mentioned above, we may restrict ourselves to real and positive $z$, i.e. $2|z| = z + z^*$. When this replacement and the equality $|v| = v$ is inserted in (20), the concurrence can be written as the expectation value of a Hamiltonian. We start by expressing $z = \langle 01|\rho|10\rangle$ and $v = \langle 00|\rho|00\rangle$ in terms of Pauli matrices,

$$z = \frac{1}{4} \text{tr} \left[ \rho (\sigma^+ \otimes \sigma^-) \right], \quad (26)$$

$$v = \frac{1}{4} \text{tr} \left[ \rho (\sigma^z - 1) \otimes (\sigma^z - 1) \right]. \quad (27)$$

Here $\sigma^\pm = (\sigma^x \pm i\sigma^y)$ denote the raising and lowering operators. Due to translational invariance, the matrix elements $z$ and $v$ are identical for any two neighboring sites. Thus, for non-zero concurrence and real $z$ we arrive at

$$C(N, p = N/2) = -\text{tr}(\rho H), \quad (28)$$

where the corresponding Hamiltonian $H$ is given by

$$H = \frac{1}{2N} \sum_{i=1}^{N} \left[ -\sigma^z_i \sigma^+_{i+1} - \sigma^y_i \sigma^y_{i+1} + \sigma^z_i \sigma^z_{i+1} + 1 \right]. \quad (29)$$

Here we have used that the magnetization per site is $\langle \sigma^z_i \rangle = 0$ in this special case of half-filling. The Hamiltonian (24) describes the Heisenberg model with nearest-neighbor interaction in an external magnetic field. (The relative sign between the $z$-coupling and the coupling in $x$- and $y$-direction does not change the physical properties of the system, as it can be absorbed by rotating the coordinate system of every second site by $\pi$ around the $z$-axis.) Note that the identity in $H$ corresponds to an overall energy shift of $1/2$. The ground state energy for the Heisenberg Hamiltonian in the limit $N \to \infty$ is well-known [13] and leads to

$$C(N \to \infty, p = N/2) = 2 \ln 2 - 1 = 0.386 \quad (30)$$

As explained below, even for the case $N = 20$ the concurrence is already very close to this value.

IV. IS THE SOLUTION WITHOUT NEIGHBORING UP-SPINS A LOCAL MAXIMUM?

The analytical solution for the maximal concurrence for any $N$ and $p$ was found in [7] by making the further restriction (ii) of no neighboring up-spins. This leads to $y = 0$ in Eq. (3), and one only needs to consider $z$. The matrix element $z$ can be written as a quadratic form in the coefficients of Eq. (6): $z = a^T Z a$, where $a$ denotes the vector with entries $a_\mu$, and $Z$ is a matrix, the dimension of which depends on $N$ and $p$. Thus, the problem of maximizing the concurrence corresponds to finding the maximal eigenvalue of $Z$, i.e.

$$C^{\text{max}}(N, p) = 2 \max_k \{ \lambda_k(Z) \}, \quad (31)$$

where $\lambda_k(A)$ denotes the $k$th eigenvalue of $A$. This diagonalization problem can be solved by the Jordan-Wigner transformation [14].

It is in general a very hard problem to prove whether the solution in [7] — we will call it OW solution from now on — is indeed optimal. In Sec. III A we showed that for $p = 2$ and $N \geq 6$ no better solution can be found, but for general $N$ and $p$ even numerical approaches are very demanding due to the many free parameters and the non-linear character of the problem. As we explain in this section, it is, however, much easier to numerically verify whether the solution in [7] is at least a local maximum of the concurrence when the restriction of no neighboring up-spins is removed.

What we basically need to do, is to expand Eq. (3) around the solution in [7]. In principle, the restriction (ii) leads to $y = 0$ and thus to $\sqrt{v} = 0$, which means that $C$ as such is not a differentiable function of the coefficients of the state. Thus, one has to be slightly more subtle than simply finding the gradient of $C$. First of all, we observe that there is a natural grouping of the coefficients according to how many up-up pairs the corresponding state contains: the maximal number is $p - 1$, the minimal 0. A useful notation is thus to split the index on the coefficients $a_\mu$ in a "group" index $\pi$ counting the number of up-up pairs and a second index $j$ distinguishing the members of each group:

$$a_\mu = a_{\pi j} = (a_{\pi})_j. \quad (32)$$
The last notation is meant to emphasize that each \( a_\pi \) can be viewed as a vector in its own right. The constraint (ii) allows only the coefficients in the 0-group to be non-vanishing, i.e. leads to \( a_\pi = (0,0,\ldots,0)^T \) for \( \pi > 0 \).

If we restrict ourselves to cases where \( \gcd(p,N) = 1 \), all normalization factors \( N_\mu \) in Eq. (8) are equal to \( 1/\sqrt{N} \), and a given coefficient’s contribution to \( y \) only depends on its group:

\[
y(a) = \frac{1}{N} \sum_\pi \pi |a_\pi|^2.
\]  
(33)

Since the number of up-up pairs gives directly the number of down-down pairs, a similar relation holds for \( v \):

\[
v(a) = \frac{1}{N} \sum_\pi (N + \pi - 2p)|a_\pi|^2 = \frac{N - 2p}{N} + y.
\]  
(34)

As for \( z \), things are naturally more complicated: \( z \) represents the mean value of \( |10\rangle\langle 01| \) and this flip of a down-up pair can at most create (or destroy) one up-up pair, i.e. there are cross-terms between \( \pi \) and \( \pi \pm 1 \). In a natural matrix notation we get:

\[
z(a) = a^T Z a
\]  
(35)

\[
= \begin{bmatrix} a_0^T & a_1^T & \ldots & a_{p-1}^T \end{bmatrix} \begin{bmatrix} Z_{00} & Z_{01} & 0 & \ldots \\ Z_{10} & Z_{11} & Z_{12} & 0 & \ldots \\ 0 & Z_{21} & Z_{22} & \ldots \\ \vdots & \vdots & \vdots & \ddots \\ Z_{p-1 \ p-2} & Z_{p-2 \ p-1} & \ldots & Z_{p-1 \ p-1} \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ \vdots \\ a_{p-1} \end{bmatrix}
\]  
(36)

where the \( Z_{\pi \pi'} \) are still matrices with indices running inside the groups. If we take the derivative of \( z \) at OW’s solution \( a = w \), we get

\[
\frac{\partial z}{\partial a_{\pi j}}(w) = 2[Z w]_{\pi j}
\]  
= \( 2\delta_{\pi 0} [Z_{00} w_0]_j + 2\delta_{\pi 1} [Z_{10} w_0]_j \)

\[
= 2\delta_{\pi 0} z(w) [w_0]_j + 2\delta_{\pi 1} [Z_{10} w_0]_j,
\]  
(37)

where have used that \( w_0 \) is an eigenvector (belonging to the largest eigenvalue) of \( Z_{00} \). Since we have the further constraint \( |a|^2 = 1 \), only the component of the gradient perpendicular to the OW solution is interesting, i.e. only the second term in Eq. (37) needs to be considered. From the \( \delta_{\pi 1} \) we see that any local first order improvement of OW’s solution can only be found by adding a small component from the space with exactly one up-up pair. Of course, when we do that \( y \) will no longer be zero, the square root in Eq. (3) will grow and this will possibly cancel the benefits we could get from \( z \) alone. A priori we should test all directions in the \( \pi = 1 \) space, but since \( y \) does not discriminate between them, the one suggested by \( z \) suffices: if \( C \) does not grow when adding an infinitesimal component along \( Z_{10} w_0 \), the solution of OW is a local maximum. The exact condition for this to happen reads:

\[
2 |Z_{10} w_0| < \sqrt{v(w)} = \sqrt{1 - \frac{2p}{N}}.
\]  
(38)

If, on the other hand, this inequality is fulfilled in the other direction, we know that OW’s solution can be improved even locally and is thus for sure not the global maximum.

In Fig. (2) we will present the results of a numerical investigation of Eq. (38) for various \( N \) and \( p \), together with the results of the non-perturbative investigation described in the following section.

V. MAPPING TO A SERIES OF HAMILTONIAN PROBLEMS

In Sec. [13] we saw how the non-linear problem of optimizing the concurrence could be stated as a linear one in the special case of \( p = N/2 \). A method which exploits this idea further has recently been introduced by Wolf et al. [11]:

\[
\begin{align*}
Z & = Z_{\pi_{\pi_1}} \\
\end{align*}
\]
The maximal value of Eq. (3) on translationally invariant states (for non-zero concurrence and \( z \) real and positive) coincides with the maximum of

\[
C(s) = z + z^* - \left( sy + \frac{1}{s} v \right),
\]

(39)

where the maximization is done over all translationally invariant states and all \( s > 0 \). To see that this holds, simply note that the minimal value of \( sy + v/s \) with respect to \( s \) is \( 2\sqrt{vy} \), which is reached for \( s = \sqrt{v/y} \). Thus, after performing first the maximization of Eq. (39) with respect to \( s \), one returns to the original problem.

If on the other hand we optimize in the opposite order, then for a given \( s \) we can generalize the method from Sec. III B and relate \( C(s) \) to the expectation value of a Hamiltonian. Explicitly we have

\[
C(s) = -\text{tr}[\rho H(s)],
\]

(40)

where

\[
H(s) = \frac{1}{2N} \sum_{i=1}^{N} \left[ -\sigma_i^x \sigma_{i+1}^x - s\sigma_i^y \sigma_{i+1}^y + \Delta(s) \left( \sigma_i^z \sigma_{i+1}^z + 1 \right) + B(s) \sigma_i^z \right].
\]

(41)

This Hamiltonian corresponds to the quantum XXZ-model with an external magnetic field \( B(s) := s - 1/s \) and an anisotropy parameter \( \Delta(s) := (s + 1/s)/2 \). For \( s = 1 \) Eq. (41) reduces to Eq. (29). The XXZ-model is completely integrable, and in principle all eigenvalues and eigenstates of the Hamiltonian (41) can be found using the Bethe ansatz. Unfortunately for general \( p \), corresponding to general magnetization, the solution is very difficult to handle even in the limit \( N \to \infty \), and we have to resort to numerical solutions.

For a given \( s \), we minimize Eq. (41) by direct diagonalization. It turns out that the dependence of the ground-state energy on \( s \) is rather simple, such that the final optimization with respect to \( s \) provides only a modest complication. In Fig. 1 we plot the results obtained for all relevant \( p \) as \( N \) ranges from 1 to 24. “Relevant” \( p \) are those with \( p \leq N/2 \), as the concurrence is identical for occupation number \( p \) and \( N - p \). For a fixed \( p \) the maximal concurrence has in general the following behavior as a function of \( N \): from the first relevant \( N = 2p \), it slightly decreases and then grows to a maximum around \( N = 3p \), after which it tends slowly to 0 as \( N \to \infty \).

FIG. 1: Maximal nearest-neighbor concurrence for \( N = 4, \ldots, 24 \). Each line and symbol type corresponds to a fixed \( p \): the left-most curve illustrates the case \( p = 1 \) and is marked by the symbol “+”. The second curve from the left shows \( p = 2 \), and so forth. The explicit legend is also given in Fig. 3. Curves with higher \( p \)’s peak at higher \( N \), the optimal value scaling roughly as \( 3p \).

In order to analyze more carefully when OW’s result is optimal, in Fig. 2 we show parts of the \( C_{\text{max}}(N) \) curves for the OW constraint of no neighboring up-spins, for the improvement via perturbation theory, and for the exact solution. As can be clearly seen, optimal states with no neighboring up-spins can be found for small numbers of sites, namely for \( N \) smaller than the value for which the concurrence has its maximum for a given \( p \). Note also that the local optimization via perturbation theory and the exact calculation always start to deviate from the OW curve at the same \( N \). This implies that when the OW state is locally optimal, it is also globally optimal.
FIG. 2: Maximal nearest-neighbor concurrence for $p = 2, \ldots, 7$ as function of the number of sites: OW result (crosses), perturbation theory (circles), and exact solution (squares). Note that the perturbation theory and the exact solution in all cases meet the OW result at the same $N$. This implies that OW’s solution is never a local maximum without being also the global maximum.

It is furthermore interesting to study the values for the optimal $s$ as a function of $N$ and $p$, see Fig. 3. These values immediately give the physical interaction that leads to the ground state with maximal nearest-neighbor concurrence. Notice that $s = 1$ for $p = N/2$, and that for any value of $p$ the optimal value of $s$ goes to infinity with $N \to \infty$. This indicates that the OW solution is indeed optimal for large $N$, and that the occurrence of neighboring up-spins for the maximization of the concurrence is a true finite size effect.

Let us also mention the exceptional case $N = 8$. In [7], no solution with a concurrence above the asymptotic value $C_{\text{max}}(N \to \infty) \approx 0.434$ was found for any $p$. Is this an artifact of the restriction to no neighboring up-spins, or a true finite size effect? Our studies show that the latter is true: we find $C_{\text{max}}(N = 8, p = 3) \approx 0.431$. Thus, together with the results presented in Table I, the occupation number $p = 2$ is shown to be optimal for $N = 8$. However, $C_{\text{max}}(N = 8, p = 2) = \sqrt{3}/4 \approx 0.433 < C_{\text{max}}(N \to \infty)$ holds — a peculiar feature of a spin chain with 8 sites.

VI. BEYOND NEAREST NEIGHBOR ENTANGLEMENT

A natural extension to the analysis done in the previous section is to examine entanglement between spins separated by at least one site. In principle, the formalism of Sec. III A can be applied to the maximization problem of the concurrence between spins separated by any number of sites. This approach yields results similar to those of Sec. III A.
For example, when maximizing the next-nearest neighbor entanglement for $p = 2$, we find that using the constraint “no next-nearest neighbors are both up”, i.e. taking $a_2 = 0$, does not decrease the concurrence for $N \geq 8$.

In this section we will treat the issue of reducing the $q$th-neighbor maximization problem of a ring with $N$ sites to a nearest-neighbor maximization problem of a ring with less than $N$ sites. In contrast to the previous sections, we will not fix the number of up-spins; we simply look for the maximum of $C$ with translational invariance and no superpositions of different $p$.

Assume first that $q$ divides $N$, i.e. $q | N$. From now on we will denote the maximal $q$th-neighbor concurrence of a ring with $N$ sites by $C^\text{max}(N, q)$. We denote by $|N\rangle^\text{opt}$ a state that reaches this value and by $p^\text{opt}$ the corresponding number of up spins.

Consider now the decomposition of the large ring into $q$ smaller rings. Each of them consists of every $q$th qubit of the large ring and has $N/q$ sites. The example of a ring with 8 sites and next-nearest-neighbor entanglement, i.e. the case $N = 8$ and $q = 2$, is illustrated in Fig. 4. The state that maximizes the nearest-neighbor concurrence of a small ring, $C^\text{max}(N/q, 1)$, will be denoted by $|N/q\rangle^\text{opt}$. The $q$-fold tensor product of this state is a candidate for the state $|N\rangle^\text{opt}$: it is translationally invariant since $T$ can be decomposed into a permutation of the set of small rings and translations within them. We thus have:

$$C(|N/q\rangle^\text{opt} \otimes \cdots \otimes |N/q\rangle^\text{opt}) \leq C^\text{max}(N, q) = C(|N\rangle^\text{opt}, q)$$  \hspace{1cm} (42)

To show than one cannot do better than using this candidate, we note that the entanglement between the first and the $q$th site of the state $|N\rangle^\text{opt}$ is calculated by tracing over all states but the first and $q$th. In particular, we trace over all but one small ring. Let us denote the state obtained by tracing out the $q - 1$ irrelevant rings by $\varrho^{(\text{s.r.})}$, i.e.

$$\varrho^{(\text{s.r.})} = \text{tr}_{\text{other rings}}|N\rangle\langle N|^{\text{opt}}.$$  \hspace{1cm} (43)

Therefore,

$$C(|N\rangle^{\text{opt}}, q) = C(\varrho^{(\text{s.r.})}, 1).$$  \hspace{1cm} (44)

Now, because the full $\varrho$ was translationally invariant, $\varrho^{(\text{s.r.})}$ is also translationally invariant. This means by definition that

$$C(\varrho^{(\text{s.r.})}, 1) \leq C^\text{max}(N/q, 1) = C(|N/q\rangle^\text{opt}, 1).$$  \hspace{1cm} (45)

Since the tensor product of Eq. (42) saturates this inequality, it must be optimal. We conclude that when $q | N$,

$$C^\text{max}(N, q) = C^\text{max}(N/q, 1).$$  \hspace{1cm} (46)

Let us now drop our assumption $q | N$ and assume that $N$ and $q$ are coprime, gcd$(N, q) = 1$. If one then tries to construct “small rings” by taking steps of $q$ sites, one will eventually visit all sites, i.e. one only finds one such ring. This simply reflects the fact that $T^q$ generates the same group of translations as $T$ does. Then it is clear that by reordering of the spins one can construct a ring on which all spins that were formerly separated by $q$ sites are now adjacent and on which translational invariance is equivalent to translational invariance with respect to the original ordering. Therefore, when gcd$(N, q) = 1$,

$$C^\text{max}(N, q) = C^\text{max}(N, 1).$$  \hspace{1cm} (47)
In general, constructing small rings by taking steps of \( q \) sites will lead to \( \text{gcd}(N, q) \) rings, each of length \( \tilde{N} = N / \text{gcd}(N, q) \). On these rings the former \( q \)th neighbors are now nearest neighbors, and an optimal state \(|N, q\rangle^{\text{opt}}\) can be constructed similarly to the \( q \mid N \) case above as a tensor product of small ring states \(|\tilde{N}, 1\rangle^{\text{opt}}\). In this way, the problem can always be reduced to the case of nearest neighbors with the result that for any \( N \) and \( q \):

\[
C^{\text{max}}(N, q) = C^{\text{max}}(N / \text{gcd}(N, q), 1). \tag{48}
\]

The method of this section naturally generalizes to other symmetry groups acting on \( N \) qubits: If we choose to optimize a given pair’s entanglement, the symmetry group will give some restrictions, but these may “factor” so that tensor product solutions of smaller problems can be applied. In the ring symmetry case, Eq. (48) shows that the reduction is maximal in the sense that there is essentially only one class of problems, namely nearest neighbors on a ring with translational symmetry. This is due to the particularly simple structure of the group of translations; in general one symmetry group may give rise to many fundamentally different optimization problems.

VII. DISCUSSION AND SUMMARY

In this paper we have studied maximal bipartite entanglement in translationally invariant spin chains with periodic boundary conditions, where our only restriction was to consider eigenstates of the \( z \) component of the total spin. We have concentrated on bipartite entanglement, as entanglement in this case is fully understood, contrary to multipartite entanglement.

Naturally, some related questions arise:

- What is the maximal entanglement between one spin and the rest of the ring?
- What is the possible structure of three- or multi-party entanglement in the ring?
- What is the optimal nearest-neighbor entanglement on a 2-dimensional lattice?

Here we will only answer the first question: states with fixed occupation number \( p \) are the eigenstates of the \( z \) component of the total spin, i.e. they are invariant under a global rotation around the \( z \)-axis, \( U = \bigotimes_{i=1}^{N} \sigma^z_i \). This leads to \( [\sigma^z, \varrho^{(1)}] = 0 \), where \( \varrho^{(1)} \) denotes the one-particle reduced density matrix, which is identical for all sites due to translational invariance. Thus, \( \varrho^{(1)} \) is diagonal, i.e. \( \varrho^{(1)} = (\mathbb{1} + s^z \sigma^z) / 2 \). Here \( s^z = \langle \sigma^z \rangle \) is the magnetization in \( z \)-direction for one site. The explicit form of the reduced density matrix is therefore

\[
\varrho^{(1)} = \frac{1}{N} \begin{bmatrix}
(N - p) & 0 \\
0 & p
\end{bmatrix}.
\]

Note that this form is independent of the choice of coefficients \( a_{\mu} \), and results only from translational invariance and the condition of fixed \( p \). The von Neumann entropy of this density matrix is a good measure for the entanglement of one qubit with the rest of the chain. Therefore, we find maximal entanglement in this sense when \( p = N/2 \).

In summary, we have investigated the maximal nearest-neighbor concurrence in translationally invariant entangled rings, where the number of up-spins \( p \) is fixed. We presented analytical results for small \( N \) and \( p = 2 \). It also turned out that the solutions in [8] can be improved by simple perturbation theory. We then used a linearized version of the concurrence, which simplified the numerical calculations, and with this method determined the maximal entanglement for any \( p \) with \( N \leq 24 \). The maximal entanglement was shown to be related to the ground state energy of an XXZ Hamiltonian. Let us emphasize our observation that a state with maximal nearest-neighbor entanglement corresponds to a Hamiltonian with only nearest-neighbor interactions. For small numbers of sites \( N \) and fixed \( p \) we gave the explicit structure of the Hamiltonian which leads to the state with maximal entanglement of nearest neighbors. We found the peculiar result that for the exceptional case \( N = 8 \) the maximal entanglement is below the entanglement in the thermodynamic limit. Finally, we reduced the problem of finding the maximal entanglement between spins which are separated by more than one site to the problem of nearest-neighbor entanglement.

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APPENDIX

Here we describe a method to find the maximal concurrence and the according state for the case \( N \geq 8 \) and \( p = 2 \). We take the normalization constraint, namely \( \sum_i a_i^2 = 1 \), into account via Lagrange multipliers.
For even $N$ we then have to solve the system of equations

\begin{align*}
    a_3 + 2a_2\lambda &= 0 , \\
    a_2 + a_4 + 2a_3\lambda &= 0 , \\
    a_3 + a_5 + 2a_4\lambda &= 0 , \\
    \ldots \\
    a_{N/2-2} + \sqrt{2}a_{N/2} + 2a_{N/2-1}\lambda &= 0 , \\
    \sqrt{2}a_{N/2-1} + 2a_{N/2}\lambda &= 0 .
\end{align*}  \quad (A.1)

where $\lambda$ is the Lagrange multiplier. For odd $N$ the last two equations in the system of equations look slightly different:

\begin{align*}
    a_{N-5}/2 + a_{N-1}/2 + 2a_{N-3}/2\lambda &= 0 , \\
    a_{N-3}/2 + a_{N-1}/2 + 2a_{N-3}/2\lambda &= 0 .
\end{align*}  \quad (A.2)

In both cases we now multiply the first equation with $a_2$, the second with $a_3$ and so on, and then add all equations. This leads to the expression

\[ C_{\text{max}} = \frac{4\lambda}{N} \]  \quad (A.3)

for the maximal concurrence. Note that this equality holds for both even and odd $N$. By inserting the first equation in the system of equations (A.1) into the second, the new one into the third, and consecutively until the last equation, one finds a polynomial equation for $\lambda$ of order $N/2 - 1$ for even $N$. By proceeding with (A.2) in the same way one arrives at a polynomial equation of order $(N-3)/2$ for odd $N$. For small $N$, these polynomial equations can be solved analytically, and for larger $N$ one can still find the zeros of the polynomial numerically.

Let us illustrate this method with a simple explicit example, namely the case $N = 8$ and $p = 2$. This is also a particularly interesting case, because in [7] in was shown that the maximal concurrence for this case (with the constraint of no two neighboring spins being up) is smaller than for the thermodynamical limit $N \to \infty$.

The system of equations for $N = 8$ and $p = 2$ is

\begin{align*}
    a_3 + 2a_2\lambda &= 0 , \\
    a_2 + \sqrt{2}a_4 + 2a_3\lambda &= 0 , \\
    \sqrt{2}a_3 + 2a_4\lambda &= 0 .
\end{align*}  \quad (A.4)

By inserting these equations successively into each other we arrive at

\[ 4\lambda^3 - 3\lambda = 0 . \]  \quad (A.5)

In order to maximize the concurrence in Eq. (A.3) we have to find the minimal solution for $\lambda$, which is $\lambda = -\sqrt{3}/2$. Therefore $C(N = 8, p = 2) = \sqrt{3}/4$. The coefficients of the optimal entangled state are then easily found to be $a_2 = \sqrt{1/6}, a_3 = \sqrt{1/2}$ and $a_4 = \sqrt{1/3}$. The results of other cases of small $N$ are given in the main text.

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