

## Entangled rings

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Consider a ring of  $N$  qubits in a translationally invariant quantum state. We ask to what extent each pair of nearest neighbors can be entangled. Under certain assumptions about the form of the state, we find a formula for the maximum possible nearest-neighbor entanglement. We then compare this maximum with the entanglement achieved by the ground state of an antiferromagnetic ring consisting of an even number of spin-1/2 particles. We find that, though the antiferromagnetic ground state typically does not maximize the nearest-neighbor entanglement relative to all other states, it does so relative to other states having zero  $z$  component of spin.

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### I. INTRODUCTION: ENTANGLEMENT SHARING

Quantum entanglement, as exemplified by the singlet state of two spin-1/2 particles,  $(1/\sqrt{2})(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$ , has been the subject of much study in recent years [1], largely because of its connection with quantum communication [2] and computation [3]. Entanglement bears some resemblance to classical correlation, but it differs in important respects, including the fact that entangled objects can violate Bell's inequality [4]. Perhaps one of the most characteristic differences is this: if two similar quantum objects are completely entangled with each other, then neither of them can be at all entangled with any other object, whereas there is no such restriction on classical correlations. This property is sometimes called the "monogamy" of entanglement. For the special case of three binary quantum objects—three qubits—a quantitative extension of this rule has been proven in terms of a measure of entanglement called the "concurrence," which takes values between zero and one: the square of the concurrence between qubits  $A$  and  $B$ , plus the square of the concurrence between qubits  $A$  and  $C$ , cannot exceed unity [5]. In other words, to the extent that qubits  $A$  and  $B$  are entangled with each other, they limit the entanglement between qubits  $A$  and  $C$ .

The present paper further explores the degree to which entanglement can be shared among a number of qubits. We focus on two closely related but distinct problems. (i) We consider a ring of  $N$  qubits in a translationally invariant quantum state and ask to what extent nearest neighbors can be entangled with each other; specifically, we ask how large the nearest-neighbor concurrence can be. Note that in this first problem there is no Hamiltonian specified; we are simply asking about the entanglement characteristics of quantum states. (ii) For our second problem we consider a particular physical system, namely a ring of  $N$  spin- $\frac{1}{2}$  particles interacting via the Heisenberg antiferromagnetic Hamiltonian, and ask whether the ground state of this system is a state of maximum nearest-neighbor entanglement. We will find that the antiferromagnetic ring maximizes entanglement within a limited set of states, but not absolutely.

In both of these problems, we are focusing on *pairwise* entanglement within a system of  $N$  particles. A number of problems with a similar focus have been considered before. Dür [6] has shown that given a system of  $N$  qubits and any

specified set of pairs of those qubits, one can design a state such that all the pairs in the chosen set are entangled and all the other pairs are not. For the specific case of three qubits, Dür *et al.* [7] have found a state that maximizes the *minimum* of the three pairwise entanglements; the concurrences for this state are all equal, the common value being  $2/3$ . Koashi *et al.* [8] have studied completely symmetric states of  $N$  qubits and have found that the maximum possible concurrence between pairs is exactly  $2/N$ . Thus in this context where all the qubits are required to be equally entangled with each other, the pairwise entanglement goes to zero in the limit of an infinite collection. Wootters [9] has considered a different problem, in which the qubits are arranged in an infinite line and only the nearest-neighbor entanglement is maximized. He found that for the infinite chain in a translationally invariant state, the nearest-neighbor concurrence does not have to be zero but can be as large as 0.434. It is not yet known whether this value is optimal. The problem we are about to address is the simplest finite version of the infinite chain problem.

There have been several other studies of entanglement in  $N$ -component systems, usually focusing on higher-order rather than pairwise entanglement [10]. Briegel and Raussendorf, in particular, have used the Ising interaction to generate interesting states exhibiting high-order entanglement [11].<sup>1</sup> All of these studies contribute to our understanding of entanglement distributed among many objects. We hope that our present results can eventually be combined with other work to construct a general theory of entanglement sharing, not limited to qubits or to any particular geometry.

### II. MAXIMIZING NEAREST-NEIGHBOR ENTANGLEMENT

We begin by recalling the definition of the concurrence [12,13] between a pair of qubits, which we will think of as

<sup>1</sup>Though Ref. [11] is similar to our work in that it relates a magnetic Hamiltonian to entanglement, the focus is quite different. For example, Ref. [11] uses the Hamiltonian dynamically to generate entanglement from an initially unentangled state, whereas we focus here on the entanglement of the ground state.

spin- $\frac{1}{2}$  particles. Let  $\rho$  be the density matrix of the pair, expressed in the standard basis  $\{|\uparrow\uparrow\rangle, |\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle, |\downarrow\downarrow\rangle\}$ . Let  $\tilde{\rho}$  be the spin-reversed density matrix, defined by  $\tilde{\rho} = (\sigma_y \otimes \sigma_y) \rho^T (\sigma_y \otimes \sigma_y)$ , where  $\sigma_y$  is the matrix  $\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$  and the superscript  $T$  indicates transposition. Then the concurrence of  $\rho$  is given by  $C = \max\{\lambda_1 - \lambda_2 - \lambda_3 - \lambda_4, 0\}$ , where the  $\lambda_i$  are the square roots of the eigenvalues of  $\rho\tilde{\rho}$  in descending order. (These eigenvalues are guaranteed to be real and non-negative even though  $\rho\tilde{\rho}$  is not necessarily Hermitian.) Concurrence is justified as a measure of entanglement by a theorem [13] showing that  $C$  is a monotonically increasing function of the entanglement of formation [14]. As we mentioned above, the values of concurrence range from zero, for an unentangled state, to one, for a completely entangled state such as the singlet state.

We imagine a set of  $N$  particles arranged in a ring, with the locations of the particles labeled by an integer  $i = 1, \dots, N$ . In defining our problem, we restrict our attention to translationally invariant pure states  $|\psi\rangle$ , that is, states that under the cyclic permutation  $i \rightarrow i+k \pmod{N}$  are changed by at most an overall phase factor. Translational invariance forces the concurrence to be the same for each pair of nearest neighbors. The problem, then, is simply to find the maximum possible value of this concurrence.<sup>2</sup> In the Appendix we show that the restriction to pure states entails no loss of generality: a translationally invariant mixed state cannot have a greater pairwise concurrence than the best pure state.

We have not yet been able to solve our problem in full. We solve instead a more tractable problem in which we limit the set of states over which the maximization is to be done. Specifically, we require our states to satisfy the following two conditions.<sup>3</sup>

1. The state  $|\psi\rangle$  of the ring is an eigenstate of the total  $z$  component of spin.

2. Neighboring particles cannot both be in the state  $|\uparrow\rangle$ . Though we are clearly leaving out many possible states, it is plausible that the maximum value we obtain for our restricted problem will not be far from the absolute maximum. This is because our two conditions tend to favor states with

<sup>2</sup>For a general, nontranslationally invariant state, one could define at least two distinct problems along similar lines: (i) maximize the *average* entanglement over all nearest-neighbor pairs, and (ii) maximize the *minimum* entanglement of all nearest-neighbor pairs (see Ref. [7]). The first of these problems could be sensitive to the measure of entanglement one is using—e.g., concurrence, squared concurrence, or entanglement of formation—even though these are all monotonic functions of each other. Problem (ii), which does not have this sensitivity, may thus be more interesting; it may also reduce to the translationally invariant problem considered here. A related, but different, generalization of our problem would be to force all the concurrences between neighboring particles to be the same, without enforcing translational invariance of the state. We insist on translational invariance simply to make the problem more manageable.

<sup>3</sup>Condition 2 breaks the symmetry between  $|\uparrow\rangle$  and  $|\downarrow\rangle$ . Our choice to use  $|\uparrow\rangle$  rather than  $|\downarrow\rangle$  in the statement of this condition is arbitrary and does not affect any of our conclusions.

high nearest-neighbor entanglement. To see this, let us consider the density matrix  $\rho$  of a pair of nearest neighbors, obtained by tracing  $|\psi\rangle\langle\psi|$  over all the other particles. Condition 1 implies that for any pair of particles, there can be no *coherent superposition* of basis states with different numbers of up spins, e.g.,  $|\downarrow\downarrow\rangle$  and  $|\downarrow\uparrow\rangle$ , because the corresponding states of the rest of the chain are orthogonal. The density matrix  $\rho$  must therefore have the following block-diagonal form:<sup>4</sup>

$$\rho = \begin{pmatrix} v & 0 & 0 & 0 \\ 0 & w & z & 0 \\ 0 & \bar{z} & x & 0 \\ 0 & 0 & 0 & y \end{pmatrix}. \quad (1)$$

One can show by direct calculation that the concurrence of this density matrix is

$$C = 2 \max\{|z| - \sqrt{vy}, 0\}. \quad (2)$$

Condition 2 implies that the matrix element  $v$  is zero, so that the neighboring-pair density matrix becomes

$$\rho = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & w & z & 0 \\ 0 & \bar{z} & x & 0 \\ 0 & 0 & 0 & y \end{pmatrix} \quad (3)$$

and the concurrence becomes simply

$$C = 2|z|. \quad (4)$$

Density matrices of the form (3) have been singled out in two recent studies as having particularly high entanglement. Specifically, Ishizaka and Hiroshima [15] have proven that such density matrices maximize entanglement for a fixed set of eigenvalues when one of the eigenvalues is zero. [They also show numerically that the form (1) is optimal when all four eigenvalues are nonzero, a result that has been proven by Verstraete *et al.* [16].] Munro *et al.* [17] have shown that certain states of the form (3) maximize concurrence for a fixed value of the purity, defined as  $\text{Tr}(\rho^2)$ . These studies suggest that our two conditions are consistent with high entanglement, but they do not guarantee that we will be able to reach the absolute maximum. Indeed, we will see below that for at least one value of  $N$ , the optimal concurrence is *not* achievable by any state satisfying our conditions. Nevertheless, our solution to the restricted problem will be useful in

<sup>4</sup>In fact translational invariance implies that the matrix elements  $w$  and  $x$  must be equal—the frequency of occurrence of  $|\uparrow\downarrow\rangle$  in the ring must be the same as that of  $|\downarrow\uparrow\rangle$ —but we will not need to use this equality in what follows.

Sec. III where we discuss antiferromagnetic rings, and it should also serve as a good starting point for future work on the complete problem.

Condition 1 forces the ring's state  $|\psi\rangle$  to have a fixed number  $p$  of up spins and a fixed number  $N-p$  of down spins, but it does not specify the value of  $p$ . Our strategy will be to fix the values of both  $N$  and  $p$  and to maximize the nearest-neighbor concurrence over all states having these values and satisfying condition 2. This problem turns out to be exactly soluble, so that one can write down an analytic formula for the maximum concurrence  $C_{max}(N,p)$ . We can then use this formula to find the optimal number of up spins, and hence the optimal concurrence, for any ring size  $N$ .

For fixed  $N$  and  $p$ , the most general state we are considering has the form

$$|\psi\rangle = \sum_{1 \leq i_1 < \dots < i_p \leq N} b_{i_1 \dots i_p} |i_1 \dots i_p\rangle, \quad (5)$$

where  $|i_1 \dots i_p\rangle$  is the state in which the particles at locations  $i_1, \dots, i_p$  have their spins up and all the other particles have their spins down. Though the above sum requires values of  $b$  only for sets of indices that are in ascending order, for convenience we define  $b$  to be symmetric in all its indices and equal to zero if any two indices have the same value. The normalization condition on the coefficients  $b$  is

$$\sum_{1 \leq i_1 < \dots < i_p \leq N} |b_{i_1 \dots i_p}|^2 = 1. \quad (6)$$

The condition of translational invariance is expressed as

$$b_{i_1 \dots i_p} = e^{ik\theta} b_{i_1+k \dots i_p+k}, \quad (7)$$

where addition is understood to be mod  $N$  and  $e^{iN\theta} = 1$ . Finally, in accordance with condition 2 above, the coefficients  $b$  must satisfy the constraint

$$b_{i_1 \dots i_p} = 0 \quad \text{if} \quad i_n - i_m = 1 \quad \text{for any} \quad n, m = 1, \dots, p. \quad (8)$$

That is, no state is allowed in which two up-spins are adjacent.

To find the concurrence between two neighboring particles, we need to find the off-diagonal element  $z$  of the two-particle density matrix as expressed in Eq. (3). Translational invariance guarantees that the value of  $z$  will be the same for each pair of nearest neighbors; we consider a specific pair at locations  $i$  and  $i+1$ . Taking the partial trace of  $|\psi\rangle\langle\psi|$  over all the other particles, we find that

$$z = \sum_{1 \leq k_2 < \dots < k_p \leq N} b_{i, k_2 \dots k_p} \bar{b}_{i+1, k_2 \dots k_p}, \quad (9)$$

so that

$$C = 2|z| = \left| \sum_{1 \leq k_2 < \dots < k_p \leq N} 2b_{i, k_2 \dots k_p} \bar{b}_{i+1, k_2 \dots k_p} \right|. \quad (10)$$

This form tells us immediately that the concurrence can be maximized by choosing the coefficients  $b$  to be real and non-negative: if we were to use complex values, then the concurrence could only be made larger, not smaller, by replacing each coefficient  $b$  by its absolute value. Let us therefore restrict our attention to such real and non-negative states. In that case, translational invariance takes the simple form

$$b_{i_1 \dots i_p} = b_{i_1+k, \dots, i_p+k}. \quad (11)$$

Thus, once the values of  $b_{1, i_2 \dots i_p}$  are fixed, all the other  $b$ 's are determined.

The condition expressed by Eq. (8), i.e., that no two up spins should be adjacent, is an awkward one to enforce directly. It is therefore helpful to relate our problem to a simpler problem that does not have this constraint. Roughly speaking, we do this by removing from the ring the site immediately to the right of each up spin. More precisely, we consider a ring of  $N-p$  particles with exactly  $p$  up spins, and we assign to every state  $|\psi\rangle$  of our original ring (every state, that is, that satisfies our conditions) a corresponding state  $|\phi\rangle$  of the smaller ring

$$|\phi\rangle = \sum_{1 \leq j_1 < \dots < j_p \leq N-p} d_{j_1 \dots j_p} |j_1 \dots j_p\rangle. \quad (12)$$

The coefficients  $d$  are defined in terms of the original coefficients  $b_{1, i_2 \dots i_p}$  with  $1 < i_2 < \dots < i_p$ . Let  $j_2 = i_2 - 1$ ,  $j_3 = i_3 - 2, \dots, j_p = i_p - (p-1)$ ; then  $d_{1, j_2 \dots j_p} \equiv \sqrt{N/(N-p)} b_{1, i_2 \dots i_p}$ . The values of the other  $d$ 's are determined by translational invariance—that is,  $d_{j_1 \dots j_p} = d_{j_1+k, \dots, j_p+k} \pmod{N-p}$ —and as before, we take  $d_{j_1 \dots j_p}$  to be symmetric under permutations of the indices and equal to zero whenever two indices have the same value. The factor  $\sqrt{N/(N-p)}$  is included in order to make  $|\phi\rangle$  normalized: translations around the ring generate fewer  $d$ 's than  $b$ 's, so that the  $d$ 's need to be larger.<sup>5</sup> Let us define a pseudoconcurrence  $C'$  of the smaller ring by analogy with Eq. (10),

$$C' = \sum_{1 \leq k_2 < \dots < k_p \leq N-p} 2d_{j, k_2 \dots k_p} \bar{d}_{j+1, k_2 \dots k_p}, \quad (13)$$

where we have omitted the absolute value sign since the  $d$ 's are all real and non-negative. Because our states of the small ring do not satisfy condition 2,  $C'$  is not the nearest-neighbor concurrence of the state  $|\phi\rangle$ . However, because of the relationship between  $d$  and  $b$ , we can use  $C'$  to find the concurrence  $C$  of our original ring,

$$C = \frac{N-p}{N} C'. \quad (14)$$

<sup>5</sup>For each collection of  $b$ 's that are equal because of translational invariance, there is a corresponding set of  $d$ 's, and the ratio of the sizes of these sets is always  $N/(N-p)$ .

Thus we want to find the maximum possible value of  $C'$  over all real and non-negative, translationally invariant states of the  $(N-p)$ -particle ring with exactly  $p$  up spins.

To do this, let us rewrite Eq. (13) in a more convenient form by introducing the creation and annihilation operators

$$a_j^\dagger = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \quad \text{and} \quad a_j = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, \quad (15)$$

which act on the particle at location  $j$  of the small ring and are expressed here in the basis  $\{|\uparrow\rangle, |\downarrow\rangle\}$ . In terms of these operators, Eq. (13) becomes simply

$$C' = 2 \langle \phi | a_{j+1}^\dagger a_j | \phi \rangle. \quad (16)$$

The value given by Eq. (16) is the same for all pairs  $\{j, j+1\}$ . We can therefore write  $C'$  as the average of this quantity over  $j$ ,

$$C' = \frac{2}{N-p} \langle \phi | \sum_{j=1}^{N-p} a_{j+1}^\dagger a_j | \phi \rangle. \quad (17)$$

Again using our assumption that the coefficients are real, we can reexpress Eq. (17) as

$$C' = - \left( \frac{1}{N-p} \right) \langle \phi | H | \phi \rangle, \quad (18)$$

where

$$H = - \sum_{j=1}^{N-p} (a_j^\dagger a_{j+1} + a_{j+1}^\dagger a_j). \quad (19)$$

In other words, a state  $|\phi\rangle$  maximizes  $C'$  if it minimizes the expectation value of the operator  $H$ , as long as this minimum is achieved with only non-negative real values of the coefficients  $d$ .

The operator  $H$  is the Hamiltonian for the one-dimensional ferromagnetic XY model; so our problem reduces to finding the lowest-energy state of this model with exactly  $p$  spins up. This is a solved problem [18]. The solution begins with the observation that the operators  $a^\dagger$  and  $a$  are not quite fermionic creation and annihilation operators, since  $[a_j, a_k] = [a_j, a_k^\dagger] = [a_j^\dagger, a_k^\dagger] = 0$  for  $j \neq k$ , whereas truly fermionic operators attached to different sites would anticommute. It is helpful to define new creation and annihilation operators  $c^\dagger$  and  $c$  that are genuinely fermionic

$$c_j = \exp \left[ i\pi \sum_{k=1}^{j-1} a_k^\dagger a_k \right] a_j, \quad (20)$$

$$c_j^\dagger = a_j^\dagger \exp \left[ -i\pi \sum_{k=1}^{j-1} a_k^\dagger a_k \right]. \quad (21)$$

In terms of the  $c$  operators, we have

$$H = - \sum_{j=1}^{N-p} (c_j^\dagger c_{j+1} + c_{j+1}^\dagger c_j) \quad \text{if } p \text{ is odd} \quad (22)$$

and

$$H = - \sum_{j=1}^{(N-p)-1} (c_j^\dagger c_{j+1} + c_{j+1}^\dagger c_j) \\ + (c_{N-p}^\dagger c_1 + c_1^\dagger c_{N-p}) \quad \text{if } p \text{ is even.} \quad (23)$$

For either odd or even  $p$ , the Hamiltonian can be diagonalized exactly, so that the system can be regarded as a collection of  $p$  independent identical fermions. For odd  $p$ , one finds that the energy eigenvalues of these fermions are  $e_m = -2 \cos[2m\pi/(N-p)]$ ,  $m=1, \dots, N-p$ , whereas for even  $p$  they are  $e_m = -2 \cos[(2m+1)\pi/(N-p)]$ ,  $m=1, \dots, N-p$ . The minimum value of  $\langle \phi | H | \phi \rangle$  is the sum of the  $p$  smallest values  $e_m$ , since in the ground state the fermions will occupy the  $p$  lowest energy levels. This sum turns out to be given by the following formula, valid for both even and odd values of  $p$ ,

$$E_{min} = - \frac{2 \sin \left( \frac{p\pi}{N-p} \right)}{\sin \left( \frac{\pi}{N-p} \right)}. \quad (24)$$

The state  $|\phi\rangle$  corresponding to this energy is the discrete version of the ground-state wave function of a set of  $p$  hard beads on a loop of wire. The coefficients  $d_{j_1 \dots j_p}$  associated with this state can be taken to be real and non-negative, and the state is translationally invariant. Thus the assumed conditions are met and we can use  $E_{min}$  to find the maximum pseudoconcurrency  $C'_{max}$  in accordance with Eq. (18),

$$C'_{max} = - \frac{1}{N-p} E_{min} = \frac{2 \sin \left( \frac{p\pi}{N-p} \right)}{(N-p) \sin \left( \frac{\pi}{N-p} \right)}. \quad (25)$$

Finally, using the relation (14), we get the maximum nearest-neighbor concurrency of our original ring of  $N$  particles,

$$C_{max}(N, p) = \frac{2 \sin \left( \frac{p\pi}{N-p} \right)}{N \sin \left( \frac{\pi}{N-p} \right)}. \quad (26)$$

Again, this is the maximum value under the following assumptions: (i) the ring has exactly  $p$  spins up, and (ii) no two up spins are adjacent.

For a given value of  $N$ , we now need to find out what value of  $p$  maximizes  $C_{max}(N, p)$ . For any fixed  $N$  it is easy enough to carry out this maximization explicitly. Consider, for example, the case  $N=7$ . In a ring of seven particles, the number  $p$  of up spins can have any of the following values without violating our condition 2:  $p=0, 1, 2$ , and  $3$ . Inserting these numbers into Eq. (26) we get the corresponding values of the concurrency:  $C=0, 0.286, 0.462$ , and  $0.286$ . Thus for a ring of seven particles it is best (under our assumptions) to have two spins up and five spins down. We have carried out

this sort of direct maximization for the first several values of the ring size  $N$ , with the following results:

$N$	2	3	4	5	6	7	8	9	10
$p_{opt}$	1	1	1	1 or 2	2	2	2	3	3
$C_{max}$	1.000	0.667	0.500	0.400	0.471	0.462	0.433	0.444	0.449

Note that though the maximum concurrence tends to decrease with increasing  $N$ , it is by no means monotonic.

It is interesting to find the limiting value of  $C_{max}$  as  $N$  goes to infinity. To do this, we write Eq. (26) in terms of  $N$  and  $\alpha \equiv p/N$ , and hold  $\alpha$  fixed as  $N$  goes to infinity. The result is

$$C_{max}(\alpha) = \frac{2}{\pi}(1-\alpha)\sin\left(\frac{\alpha\pi}{1-\alpha}\right). \quad (27)$$

This equation gives the maximum nearest-neighbor concurrence (under our assumptions) for an infinite chain of spin- $\frac{1}{2}$  particles in which the overall density of up spins is  $\alpha$ . It is reassuring that this formula is identical to the one obtained in Ref. [9], which considered only infinite chains. Differentiating Eq. (27), one finds that the optimal value of  $\alpha$  is 0.300 844, for which  $C_{max} = 0.434 467$ . This number is thus our candidate for the maximum nearest-neighbor concurrence of an infinite chain of qubits (as in Ref. [9]). Note that, perhaps surprisingly, for rings of five and eight particles, the maximum values of  $C$  as given in the above table are *smaller* than the limiting value for an infinite chain. This is no doubt because in these cases one is near the ‘‘borderline’’ between two different values of  $p_{opt}$ , and neither is particularly good. This fact also suggests that the cases  $N=5$  and  $N=8$  are the best places to look for examples in which the maximum concurrence is *not* achieved by a state satisfying our conditions.

Indeed, by relaxing condition 2, one *can* achieve higher entanglement for  $N=5$ . The state

$$|\psi\rangle = \frac{1}{\sqrt{5}}\{\sin\theta[|\uparrow\uparrow\downarrow\downarrow\rangle + \dots] + \cos\theta[|\uparrow\downarrow\uparrow\downarrow\rangle + \dots]\}, \quad (28)$$

where the ellipses stand for all translations of the given basis state, has a nearest-neighbor concurrence  $C=0.468$  when  $\theta=0.302$ , which is better than the value shown in the above table. We have looked for similar numerical improvements for  $N=6, 7, 8, 9$ , and  $10$ , in each case relaxing condition 2 but preserving condition 1, and we have found none (not even for  $N=8$ ). For  $N=4$  we have removed both conditions 1 and 2 and have found no numerical improvement. Finally, for  $N=3$  it follows from Refs. [7] and [8] that our result is optimal without these conditions. Thus it is conceivable that our formula gives the true maximum for many values of  $N$ , though it does not do so for all values. In any case, it gives us a lower bound on the maximum nearest-neighbor concurrence, which we will be able to use in the following section.

To close this section, we write down explicitly the neighboring-pair density matrix for our optimal state of the infinite chain. In the form (3), the matrix elements  $w$  and  $x$  must both be equal to  $\alpha$ , the density of up spins. This is because every up-spin is isolated, so that the probability of the pair state  $|\uparrow\downarrow\rangle$  is the same as the probability that the first particle has its spin up, and similarly for the probability of  $|\downarrow\uparrow\rangle$ . We already have the value of  $z$ , namely, half the concurrence; so the density matrix is

$$\rho = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0.301 & 0.217 & 0 \\ 0 & 0.217 & 0.301 & 0 \\ 0 & 0 & 0 & 0.398 \end{pmatrix}. \quad (29)$$

This matrix is not quite one of the special states identified by Munro *et al.* [17], which maximize entanglement for a fixed purity of the density matrix. Such a state would have all three of the nonzero diagonal elements equal to  $1/3$ . The fact that it is not the same shows that our problem is not equivalent to the fixed-purity problem. Nevertheless, it is interesting that the two results are as similar as they are.

### III. ENTANGLEMENT IN AN ANTIFERROMAGNETIC RING

Though we introduced an effective Hamiltonian in order to solve the preceding problem, the problem itself did not specify any Hamiltonian. We now consider a more concrete physical model of a ring of  $N$  qubits, namely, an antiferromagnetic ring of spin- $\frac{1}{2}$  particles in which neighboring particles interact via the Heisenberg Hamiltonian

$$H = \sum_i^N \vec{\sigma}_i \cdot \vec{\sigma}_{i+1}. \quad (30)$$

Here  $\vec{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$  is the vector of Pauli matrices and, as before, the sum  $i+1$  is understood to wrap around to 1 when  $i=N$ . This model has been studied extensively over many decades, much of the foundational work having been done by Bethe in the early days of quantum mechanics [19]. In the spirit of Sec. II we ask a new question about the model: does the ground state maximize the nearest-neighbor entanglement? We restrict our attention to rings with an *even* number of particles, partly because the calculation is considerably simpler in that case, and partly because the symmetry of the even- $N$  ground state suggests an interesting refinement of our question, as we will see shortly.

For the antiferromagnetic ring there is good reason to expect a connection between minimizing the energy and maximizing the entanglement. Contrary to what one would expect classically, the ground state is not simply the alternating state  $|\uparrow\downarrow\uparrow\downarrow\cdots\rangle$ . Though this alternating state minimizes the energy due to the  $\sigma_z$  part of the Hamiltonian, it does not do so well for the  $\sigma_x$  and  $\sigma_y$  parts. By contrast, the ground state for  $N=2$ , which is the singlet state

$$|\psi\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle), \quad (31)$$

treats all directions of space equivalently since it is rotationally invariant. Intuitively, one expects that for a ring of  $N$  particles, each pair of nearest neighbors is ‘‘trying’’ to be in the singlet state in order to minimize its own energy but is thwarted to some extent by the similar efforts of neighboring pairs. Now, the singlet state is maximally entangled; so in a certain sense each pair of nearest neighbors, by trying to minimize its energy, is also trying to be entangled. We want to see whether the pairs go as far in this direction as they possibly could, that is, whether they in fact maximize the nearest-neighbor entanglement. Though we do not yet know the maximum possible value of this entanglement (because of the extra conditions we imposed on our states in Sec. II), we can nevertheless use the result of Sec. II as a benchmark for evaluating the entanglement of the antiferromagnetic ring. For example, if the nearest-neighbor concurrence of the infinite chain is less than 0.434467, we know that the entanglement is not maximal.

We begin by invoking some basic facts about the ground state of an antiferromagnetic ring with an even number of particles [20]: it is translationally invariant, and it is an eigenstate of the total  $z$  component of spin with eigenvalue zero. These properties guarantee that the density matrix of each pair of neighboring particles has the form

$$\rho = \begin{pmatrix} v & 0 & 0 & 0 \\ 0 & w & z & 0 \\ 0 & \bar{z} & w & 0 \\ 0 & 0 & 0 & v \end{pmatrix}. \quad (32)$$

Let  $E$  be the ground-state energy of the system, so that  $E/N$  is the contribution from a single pair:  $E/N = \text{Tr}[\rho(\vec{\sigma} \cdot \vec{\sigma})]$ . We now reexpress the energy  $E/N$  in terms of the matrix elements of  $\rho$ . The matrix  $\vec{\sigma} \cdot \vec{\sigma}$ , written explicitly in the standard basis, is

$$\vec{\sigma} \cdot \vec{\sigma} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 2 & 0 \\ 0 & 2 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \quad (33)$$

Thus

$$E/N = \text{Tr}[\rho(\vec{\sigma} \cdot \vec{\sigma})] = 2(v - w + 2 \text{Re } z) = 4(v + \text{Re } z) - 1, \quad (34)$$

where we have used the fact that  $\text{Tr } \rho = 1$ .

It is useful at this point to write the matrix elements  $v$  and  $z$  in terms of the coefficients that define the ring's state  $|\psi\rangle$ . Just as in Sec. II, we can write  $|\psi\rangle$  as

$$|\psi\rangle = \sum_{1 \leq i_1 < \cdots < i_p \leq N} b_{i_1 \dots i_p} |i_1 \dots i_p\rangle, \quad (35)$$

where  $p$  now has the specific value  $N/2$ . And just as before, we have

$$z = \sum_{1 \leq k_2 < \cdots < k_p \leq N} b_{i_1 k_2 \dots k_p} \bar{b}_{i_1+1, k_2 \dots k_p}. \quad (36)$$

The corresponding expression for the matrix element  $v$  is

$$v = \sum_{1 \leq k_3 < \cdots < k_p \leq N} |b_{i_1, i_1+1, k_3 \dots k_p}|^2. \quad (37)$$

Note that changes in the phases of the coefficients  $b$  do not affect  $v$ , though they do affect  $z$ . In order to minimize the energy as given in Eq. (34), we want to choose these phases so that  $\text{Re } z$  is as negative as possible. For a fixed set of absolute values of the  $b$ 's, this can be done by letting all the  $b$ 's be real, with alternating signs given by

$$\text{sign of } b_{i_1 \dots i_p} = (-1)^{i_1 + \cdots + i_p}, \quad (38)$$

in which case every term of Eq. (36) is negative or zero. Thus for the ground state of this system, we can write the energy per particle as

$$E/N = 4(v - |z|) - 1. \quad (39)$$

Now, recall that the concurrence of a density matrix of the form (32) is [Eq. (2)]

$$C = \max\{2(|z| - v), 0\}. \quad (40)$$

We thus arrive at the following expression for the concurrence  $C_{gs}$  of the ground state of this system, assuming (as is the case) that the ground-state energy is sufficiently negative to make  $C_{gs}$  positive.

$$C_{gs} = -\frac{1}{2}[(E/N) + 1]. \quad (41)$$

This simple relationship depends on the fact that the number of particles in the ring is even. If  $N$  were odd, the pair density matrix would not have the form (32) and its concurrence would most likely not be a simple function of the energy alone.

The ground-state energies of antiferromagnetic rings have been computed for many values of  $N$  [20,21], including the limiting case  $N \rightarrow \infty$  [22]. From these results and Eq. (41) we can immediately write down the concurrences. The following table shows the values of  $C_{gs}$  for several values of  $N$ , along with corresponding values of  $C_{max}$  that we computed in Sec. II. The Figure 0.386 appearing in the table as the concurrence of the ground state of the infinite chain can be written exactly as  $2 \ln 2 - 1$ .

$N$	2	4	6	8	10	...	$\infty$
$-E/N$	3.000	2.000	1.868	1.825	1.806	...	1.773
$C_{gs}$	1.000	0.500	0.434	0.412	0.403	...	0.386
$C_{max}$	1.000	0.500	0.471	0.433	0.449	...	0.434

Thus, though for very small rings the antiferromagnetic ground states are as entangled as the states we found in Sec. II, for larger rings they fall short. We can therefore conclude that the ground state of an antiferromagnetic ring does not in general maximize nearest-neighbor entanglement.

There is, however, a more limited sense in which these ground states do maximize entanglement; this is the refinement we mentioned earlier. Let us restrict our attention to the set of states which, like the ground state, are translationally invariant and have zero total  $z$  component of spin. We will call such states ‘‘balanced.’’ We now show that the antiferromagnetic ground state maximizes entanglement within the set of balanced states.

Let us divide the set of all balanced states into equivalence classes, two states being called equivalent if their coefficients  $b_{i_1 \dots i_p}$  in Eq. (35) agree in magnitude, differing only in their phases. Of all the states in a given equivalence class, none has a greater nearest-neighbor concurrence than the unique state in that class for which the phases are given by Eq. (38). This is because, as in the case of the ground state, such phases allow perfect constructive interference in Eq. (36). To put it in symbols,  $C(\psi) \leq C(\psi_0)$ , where  $|\psi\rangle$  is a general balanced state and  $|\psi_0\rangle$  is the state obtained from  $|\psi\rangle$  by adjusting the phases of the  $b$ 's in accordance with Eq. (38). Now, for  $|\psi_0\rangle$ , the expectation value of the energy  $\langle \psi_0 | H | \psi_0 \rangle$  is given by the same expression as in Eq. (39)

$$\frac{1}{N} \langle \psi_0 | H | \psi_0 \rangle = 4(v - |z|) - 1. \quad (42)$$

The concurrence of  $|\psi_0\rangle$  is given by Eq. (40), so we have

$$\begin{aligned} C(\psi) \leq C(\psi_0) &= \max \left\{ -\frac{1}{2} \left[ \frac{1}{N} \langle \psi_0 | H | \psi_0 \rangle + 1 \right], 0 \right\} \\ &\leq \max \left\{ -\frac{1}{2} [(E/N) + 1], 0 \right\} = C_{gs}. \end{aligned} \quad (43)$$

The last inequality comes from the fact that the ground state minimizes the expectation value of the energy. We have thus shown that no balanced state has a nearest-neighbor concurrence larger than that of the ground state.

For comparison with Eq. (29), it is interesting to write down explicitly the neighboring-pair density matrix for the ground state of an infinite antiferromagnetic chain. This density matrix is uniquely determined by the value of the concurrence,  $C = 2 \ln 2 - 1$ , and by the fact that the state is rotationally invariant (the latter condition implies that  $|z| + v = w$ ). One finds that

$$\rho = \begin{pmatrix} 0.102 & 0 & 0 & 0 \\ 0 & 0.398 & -0.295 & 0 \\ 0 & -0.295 & 0.398 & 0 \\ 0 & 0 & 0 & 0.102 \end{pmatrix}. \quad (44)$$

If we think of the spins of the antiferromagnetic chain as ‘‘trying’’ to maximize their entanglement, then evidently they are using a rather different strategy than the one we used in Sec. II. There is no longer any prohibition against neighboring up spins. Indeed the presence of such up-spin pairs in the antiferromagnetic chain allows the off-diagonal element  $z$  to have a larger magnitude than in Eq. (29), which is good for entanglement. On the other hand, the presence of such pairs also forces the matrix element  $v = \langle \uparrow \uparrow | \rho | \uparrow \uparrow \rangle$  to be nonzero, which is what reduces the concurrence to a value less than our best value of Sec. II.

Shortly after the first version of the present paper appeared, Arnesen *et al.* reported on related work on antiferromagnetic and ferromagnetic chains at nonzero temperatures and in nonzero magnetic fields [23]. Their work is complementary to ours in that it is primarily numerical and emphasizes the temperature and field dependence of the nearest-neighbor entanglement rather than the entanglement of the ground state.

#### IV. CONCLUSIONS

We have obtained two main results. First, for translationally invariant rings of  $N$  qubits, we have found values of the nearest-neighbor concurrences that we know to be achievable and that for some values of  $N$  appear to be optimal. At the least, they are lower bounds on the maximum possible concurrences. Second, we have found that the ground state of an antiferromagnetic ring with an even number of particles typically does not maximize the nearest-neighbor concurrence over all states, but that it does achieve such a maximum over the set of translationally invariant states with no net spin in the  $z$  direction. This set of ‘‘balanced’’ states includes all the eigenstates of total spin with eigenvalue zero; so we can also say that the ground state maximizes  $C$  relative to all the spin-0, or rotationally invariant states.

Putting Secs. II and III together, we can conclude that whatever the maximum-concurrence states may be, they are certainly not balanced. In other words, for maximizing concurrence it is best to have one direction of spin favored over the opposite direction. This is perhaps counterintuitive, since a maximally unbalanced state such as  $|\uparrow \uparrow \uparrow \dots\rangle$  is not entangled at all.

The subject of Sec. III represents an unusual mix: one does not often associate entanglement with energy minimization. One might wonder whether the entanglement-maximization property of antiferromagnetic rings, limited though it is, is a special case of a more general connection between energy and entanglement. Do physical systems tend to favor entangled states over unentangled states? In a straightforward interpretation of this question, the answer would seem to be no. *Ferromagnetic* systems, for example, have ground states in which the spins are completely unen-

tangled. Perhaps one could identify a special class of Hamiltonians with interesting entanglement-maximizing properties, but at present it is not clear how large such a class might be.

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### APPENDIX: TRANSLATIONALLY INVARIANT MIXED STATES

In the main part of this paper we assumed that our rings were in pure states. But one could also consider translationally invariant mixed states. We now show that no such state could have a greater nearest-neighbor entanglement than the best translationally invariant pure state.

Let  $\rho$  be a mixed state of a ring of  $N$  qubits. It is translationally invariant in the sense that it is unchanged under a permutation of basis states that corresponds to a translation. (E.g., in a one-step translation for  $N=7$ , the basis state  $|0100111\rangle$  becomes  $|1010011\rangle$ .) The state  $\rho$  typically can be decomposed into pure states in many ways; we consider any such decomposition

$$\rho = \sum_k |\psi_k\rangle\langle\psi_k|, \quad (\text{A1})$$

where each state vector  $|\psi_k\rangle$  is *subnormalized* so that  $|\langle\psi_k|\psi_k\rangle|^2$  is the probability with which  $|\psi_k\rangle$  appears in the mixture.

There is no guarantee that each  $|\psi_k\rangle$  is itself translationally invariant. However, we can create from Eq. (A1) a new decomposition in which all the states are translationally invariant. First, we enlarge the decomposition (A1) by averaging over all  $N$  translations:

$$\rho = \frac{1}{N} \sum_{k,m} |\psi_{km}\rangle\langle\psi_{km}|, \quad (\text{A2})$$

where  $|\psi_{km}\rangle$  is obtained from  $|\psi_k\rangle$  by an  $m$ -step translation. Next, we define a set of translationally invariant pure states  $|\phi_{kn}\rangle$  as follows:

$$|\phi_{kn}\rangle = \frac{1}{N} \sum_m e^{(2\pi i/N)mn} |\psi_{km}\rangle, \quad n=0, \dots, N-1. \quad (\text{A3})$$

Note that each  $|\phi_{kn}\rangle$  has a norm less than or equal to one. Finally, we construct the following mixture, which is another decomposition of  $\rho$ :

$$\begin{aligned} \sum_{k,n} |\phi_{kn}\rangle\langle\phi_{kn}| &= \frac{1}{N^2} \sum_{k,n,m,m'} e^{(2\pi i/N)n(m-m')} |\psi_{km}\rangle\langle\psi_{km'}| \\ &= \frac{1}{N} \sum_{k,m} |\psi_{km}\rangle\langle\psi_{km}| = \rho. \end{aligned} \quad (\text{A4})$$

We may write this decomposition in a more standard form by defining normalized state vectors  $|\Phi_{kn}\rangle$  such that  $|\phi_{kn}\rangle = \sqrt{p_{kn}} |\Phi_{kn}\rangle$ . Then we have

$$\rho = \sum_{k,n} p_{kn} |\Phi_{kn}\rangle\langle\Phi_{kn}|. \quad (\text{A5})$$

Thus  $\rho$  can always be written as a mixture of translationally invariant pure states, namely, the states  $|\Phi_{kn}\rangle$ .

We now need to find the concurrence of a pair of neighboring particles when the whole ring is in the state  $\rho$ . Let  $\rho_{pair}$  be the density matrix of such a pair, obtained by tracing over the rest of the system, which we call  $R$ .

$$\rho_{pair} = \text{Tr}_R \rho = \sum_{k,n} p_{kn} \text{Tr}_R |\Phi_{kn}\rangle\langle\Phi_{kn}|. \quad (\text{A6})$$

Concurrence is a convex function on the set of density matrices, so we have

$$\begin{aligned} C(\rho_{pair}) &= C\left(\sum_{k,n} p_{kn} \text{Tr}_R |\Phi_{kn}\rangle\langle\Phi_{kn}|\right) \\ &\leq \sum_{k,n} p_{kn} C(\text{Tr}_R |\Phi_{kn}\rangle\langle\Phi_{kn}|). \end{aligned} \quad (\text{A7})$$

The quantity  $C(\text{Tr}_R |\Phi_{kn}\rangle\langle\Phi_{kn}|)$  is the concurrence of the pair of qubits when the whole ring is in the pure state  $|\Phi_{kn}\rangle$ . The nearest-neighbor concurrence for  $\rho$  is thus no larger than the average of the nearest-neighbor concurrences for a set of translationally invariant pure states. Therefore, one of these pure states must yield a concurrence at least as large as the one determined by  $\rho$ . In other words, no translationally invariant mixed state can have a larger pairwise entanglement than the best translationally invariant pure state.

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