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Entangled Chains

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ABSTRACT. Consider an infinite collection of qubits arranged in a line, such that every pair of nearest neighbors is entangled: an "entangled chain." In this paper we consider entangled chains with translational invariance and ask how large one can make the nearest neighbor entanglement. We find that it is possible to achieve an entanglement of formation equal to 0.285 ebits between each pair of nearest neighbors, and that this is the best one can do under certain assumptions about the state of the chain.

1. Introduction: Example of an entangled chain

Quantum entanglement has been studied for decades, first because of its importance in the foundations of quantum mechanics, and more recently for its potential technological applications as exemplified by a quantum computer [**1**]. The new focus has led to a quantitative theory of entanglement [**2, 3, 4**] that, among other things, allows us to express analytically the degree of entanglement between simple systems [**5**]. This development makes it possible to pose new quantitative questions about entanglement that could not have been raised before and that promise fresh perspectives on this remarkable phenomenon. In this paper I would like to raise and partially answer such a question, concerning the extent to which a collection of binary quantum objects (qubits) can be linked to each other by entanglement.

Imagine an infinite string of qubits, such as two-level atoms or the spins of spin-1/2 particles. Let us label the locations of the qubits with an integer j that runs from negative infinity to positive infinity. I wish to consider special states of the string, satisfying the following two conditions: (i) each qubit is entangled with its nearest neighbors; (ii) the state is invariant under all translations, that is, under transformations that shift each qubit from its original position j to position $j+n$ for some integer n. Let us call a string of qubits satisfying the first condition an entangled chain, and if it also satisfies the second condition, a uniform entangled chain. Note that each qubit need not be entangled with any qubits other than its two nearest neighbors. In this respect an entangled chain is like an ordinary chain, whose links are directly connected only to two neighboring links. By virtue of the translational invariance, the degree of entanglement between nearest neighbors in a uniform entangled chain must be constant throughout the chain. The main

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question I wish to pose is this: How large can the nearest-neighbor entanglement be in a uniform entangled chain?

This problem belongs to a more general line of inquiry about how entanglement can be shared among more than two objects. Some work on this subject has been done in the context of the cloning of entanglement [**6**–**11**], where one finds limits on the extent to which entanglement can be copied. In a different setting not particularly involving cloning, one finds an inequality bounding the amount of entanglement that a single qubit can have with each of two other qubits [**12**]. One can imagine more general "laws of entanglement sharing" that apply to a broad range of configurations of quantum objects. The present work provides further data that might be used to discover and formulate such laws. The specific problem addressed in this paper could also prove relevant for analyzing models of quantum computers in which qubits are arranged along a line, as in an ion trap [**13**]. The infinite chain can be thought of as an idealization of such a computer. Moreover, the analysis of our question turns out to be interesting in its own right, being related, as we will see, to a familiar problem in many-body physics.

To make the question precise we need a measure of entanglement between two qubits. We will use a reasonably simple and well-justified measure called the "concurrence," which is defined as follows [**5**].

Consider first the case of pure states. A general pure state of two qubits can be written as

$$|\psi\rangle = \alpha|00\rangle + \beta|01\rangle + \gamma|10\rangle + \delta|11\rangle. \tag{1.1}$$

One can verify that such a state is factorizable into single-qubit states—that is, it is unentangled—if and only if $\alpha\delta = \beta\gamma$. The quantity $C = 2\,|\alpha\delta - \beta\gamma|$, which ranges from 0 to 1, is thus a plausible measure of the degree of entanglement. We take this expression as the definition of concurrence for a pure state of two qubits. For mixed states, we define the concurrence to be the greatest convex function on the set of density matrices that gives the correct values for pure states [**14**].

Though this statement defines concurrence, it does not tell us how to compute it for mixed states. Remarkably, there exists an explicit formula for the concurrence of an arbitrary mixed state of two qubits [**5**]: Let ρ be the density matrix of the mixed state, which we imagine expressed in the standard basis $\{|00\rangle, |01\rangle, |10\rangle, |11\rangle\}$. Let $\tilde{\rho}$, the "spin-flipped" density matrix, be $(\sigma_y \otimes \sigma_y)\rho^*(\sigma_y \otimes \sigma_y)$, where the asterisk denotes complex conjugation in the standard basis and σ_y is the matrix $\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$. Finally, let $\lambda_1, \lambda_2, \lambda_3, \lambda_4$ be the square roots of the eigenvalues of $\rho\tilde{\rho}$ in descending order—one can show that these eigenvalues are all real and non-negative. Then the concurrence of ρ is given by the formula

$$C(\rho) = \max\{\lambda_1 - \lambda_2 - \lambda_3 - \lambda_4, 0\}. \tag{1.2}$$

The best justification for using concurrence as a measure of entanglement comes from a theorem [**5**] showing that concurrence is a monotonically increasing function of the "entanglement of formation," which quantifies the non-local resources needed to create the given state [**4**].[1] As mentioned above, the values of C range from zero

[1] One can define the entanglement of formation as follows. Let ρ be a mixed state of a pair of quantum objects, to be shared between two separated observers who can communicate with each other only via classical signals. The entanglement of formation of ρ is the asymptotic number of singlet states the observers need, per pair, in order to create a large number of pairs in *pure*

to one: an unentangled state has $C = 0$, and a completely entangled state such as the singlet state $\frac{1}{\sqrt{2}}(|01\rangle - |10\rangle)$ has $C = 1$. Our problem is to find the greatest possible nearest-neighbor concurrence of a uniform entangled chain. At the end of the calculation we can easily re-express our results in terms of entanglement of formation.

Another issue that needs to be addressed in formulating our question is the meaning of the word "state" as applied to an infinite string of qubits; in particular we need to discuss how such a state is to be normalized. Formally, we can define a state of our system as follows. A state w of the infinite string is a function that assigns to every finite set S of integers a normalized (*i.e.*, trace one) density matrix $w(S)$, which we interpret to be the density matrix of the qubits specified by the set S; moreover the function w must be such that if S_2 is a subset of S_1, then $w(S_2)$ is obtained from $w(S_1)$ by tracing over the qubits whose labels are not in S_2. This formal definition is perfectly sensible but somewhat bulky in practice. In what follows we will usually specify states of the string more informally when it is clear from the informal specification how to generate the density matrix of any finite subset of the string. We will also usually use the symbol ρ instead of $w(S)$ to denote the density matrix of a pair of nearest neighbors.

It is not immediately obvious that there exists even a single example of an entangled chain. Note, for example, that the limit of a Schrödinger cat state—an equal superposition of an infinite string of zeros with an infinite string of ones—is not an entangled chain. In the cat state, the reduced density matrix of a pair of neighboring qubits is an incoherent mixture of $|00\rangle$ and $|11\rangle$, which exhibits a classical correlation but no entanglement. (Note, by the way, that our informal statement "an equal *superposition* of an infinite string of zeros with an infinite string of ones," specifies exactly the same state as if we had taken an incoherent *mixture* of these two infinite strings: no finite set of qubits contains information about the phase of the superposition.)

We can, however, construct a simple example of an entangled chain in the following way. Let w_0 be the state such that for each *even* integer j, the qubits at sites j and $j+1$ are entangled with each other in a singlet state. We can write this state informally as[2]

(1.3)
$$\cdots\otimes\left(\frac{|0\rangle_{-2}|1\rangle_{-1} - |1\rangle_{-2}|0\rangle_{-1}}{\sqrt{2}}\right)\otimes\left(\frac{|0\rangle_0|1\rangle_1 - |1\rangle_0|0\rangle_1}{\sqrt{2}}\right)\otimes\left(\frac{|0\rangle_2|1\rangle_3 - |1\rangle_2|0\rangle_3}{\sqrt{2}}\right)\otimes\cdots$$

states whose average density matrix is ρ. (This is conceptually different from the *regularized* entanglement of formation, which measures the cost of creating many copies of the *mixed* state ρ [**15**]. However, it is conceivable that the two quantities are identical.) Entanglement of formation is conventionally measured in "ebits," and for a pair of binary quantum objects it takes values ranging from 0 to 1 ebit.

[2]Alternatively, we can characterize the state w_0 according to our formal definition by specifying the density matrix of each finite collection of qubits: Let S define such a collection. Then for each even integer j such that both j and $j+1$ are in S, the corresponding pair of qubits is in the singlet state; all other qubits (*i.e.*, the unpaired ones) are in the completely mixed state $\begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix}$, and the full density matrix $w(S)$ is obtained by taking the tensor product of the pair states and single-qubit states.

The state w_0 is not an entangled chain because the qubits are not entangled with both of their nearest neighbors: qubits at even-numbered locations are not entangled with their neighbors on the left. However, if we let w_1 be the state obtained by translating w_0 one unit to the left (or to the right—the result is the same), and let w be an equal mixture of w_0 and w_1—that is, $w = (w_0 + w_1)/2$—then w is a uniform entangled chain, as we now show.

That w is translationally invariant follows from the fact that both w_0 and w_1 are invariant under *even* displacements and that they transform into each other under odd displacements. Thus we need only show that neighboring states are entangled. For definiteness let us consider the qubits in locations $j = 1$ and $j = 2$. In the state w_0, the density matrix for these two qubits is

$$\rho^{(0)} = \begin{pmatrix} \frac{1}{4} & 0 & 0 & 0 \\ 0 & \frac{1}{4} & 0 & 0 \\ 0 & 0 & \frac{1}{4} & 0 \\ 0 & 0 & 0 & \frac{1}{4} \end{pmatrix}, \tag{1.4}$$

that is, the completely mixed state. (The two qubits are from distinct singlet pairs.) The density matrix of the same two qubits in the state w_1 is

$$\rho^{(1)} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & \frac{1}{2} & 0 \\ 0 & \frac{1}{2} & \frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \tag{1.5}$$

that is, the singlet state. In the state w, the qubits are in an equal mixture of these two density matrices, which is

$$\rho = (\rho^{(0)} + \rho^{(1)})/2 = \begin{pmatrix} \frac{1}{8} & 0 & 0 & 0 \\ 0 & \frac{3}{8} & \frac{1}{4} & 0 \\ 0 & \frac{1}{4} & \frac{3}{8} & 0 \\ 0 & 0 & 0 & \frac{1}{8} \end{pmatrix}. \tag{1.6}$$

It is easy to compute the concurrence of this density matrix, because $\tilde{\rho}$ is the same as ρ itself. The values λ_i in this case are the eigenvalues of ρ, which are $\frac{5}{8}, \frac{1}{8}, \frac{1}{8}, \frac{1}{8}$. The concurrence is therefore $C = \frac{5}{8} - \frac{1}{8} - \frac{1}{8} - \frac{1}{8} = \frac{1}{4}$. This same value of the concurrence applies to any other pair of neighboring qubits in the string because of the translational invariance. The fact that the concurrence is non-zero implies that neighboring qubits are entangled, so that the state w is indeed an entangled chain. For uniform entangled chains, we will call the common value of C for neighboring qubits the concurrence of the chain. Thus in the above example the concurrence of the chain is $\frac{1}{4}$.

As we will see, it is possible to find uniform entangled chains with greater concurrence. Let $C_{\max}$ be the least upper bound on the concurrences of all uniform entangled chains. We would like to find this number. We know that $C_{\max}$ is no larger than 1, since concurrence never exceeds 1. In fact we can quickly get a somewhat better upper bound, using the following fact: when a qubit is entangled with each of two other qubits, the sum of the squares of the two concurrences is less than or equal to one [**12**]. In a uniform entangled chain, each qubit must be equally entangled with its two nearest neighbors; so the concurrence with each of them cannot exceed $1/\sqrt{2}$. Thus, so far what we know about $C_{\max}$ is this:

$$1/4 \le C_{\max} \le 1/\sqrt{2}. \tag{1.7}$$

This is still a wide range. Most of the rest of this paper is devoted to getting a better fix on $C_{\max}$ by explicitly constructing entangled chains.

2. Building chains out of blocks

Using the above example as a model, we will use the following construction to generate other uniform entangled chains. (1) Break the string into blocks of n qubits, and define a state w_0 in which each block is in the same n-qubit state $|\xi\rangle$; that is, w_0 is a tensor product of an infinite number of copies of $|\xi\rangle$. (In the above example n had the value 2 and $|\xi\rangle$ was the singlet state.) (2) Define w_k, $k = 1, \ldots, n-1$, to be the state obtained by shifting w_0 to the left by k units. (3) Let the final state w be the average $(w_0 + \cdots + w_{n-1})/n$. A state generated in this way will automatically be translationally invariant. In order that the chain have a large concurrence, we will need to choose the state $|\xi\rangle$ carefully. Finding an optimal $|\xi\rangle$ and proving that it is optimal may turn out to be a difficult problem. In this paper I will choose $|\xi\rangle$ according to a strategy that makes sense and may well be optimal but is not proven to be so.

In the final state w, each pair of neighboring qubits has the same density matrix because of the translational invariance. Our basic strategy for choosing $|\xi\rangle$, described below, is designed to give this neighboring-pair density matrix the following form:

$$\rho = \begin{pmatrix} \rho_{11} & 0 & 0 & 0 \\ 0 & \rho_{22} & \rho_{23} & 0 \\ 0 & \rho_{32} & \rho_{33} & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}. \tag{2.1}$$

(The ordering of the four basis states is the one given above: $|00\rangle, |01\rangle, |10\rangle, |11\rangle$.) One can show that the concurrence of such a density matrix is simply

$$C = 2|\rho_{23}|. \tag{2.2}$$

Besides making the concurrence easy to compute, the form (2.1) seems a reasonable goal because it picks out a specific kind of entanglement, namely, a coherent superposition of $|01\rangle$ and $|10\rangle$, and limits the ways in which this entanglement can be contaminated or diluted by being mixed with other states. In particular, the form (2.1) does not allow contamination by an orthogonal entangled state of the form $\alpha|00\rangle + \beta|11\rangle$—orthogonal entangled states when mixed together tend to cancel each other's entanglement—or by the combination of the two unentangled states $|00\rangle$ and $|11\rangle$. If the component ρ_{44} were not equal to zero and the form were otherwise unchanged, the concurrence would be $C = \max\{2(|\rho_{23}| - \sqrt{\rho_{11}\rho_{44}}), 0\}$; so it is good to make either ρ_{11} or ρ_{44} equal to zero if this can be done without significantly reducing ρ_{23}. We have chosen to make ρ_{44} equal to zero.

As it happens, one can guarantee the form (2.1) for the density matrix of neighboring qubits by imposing the following three conditions on the n-qubit state $|\xi\rangle$: (i) $|\xi\rangle$ is an eigenstate of the operator that counts the number of qubits in the state $|1\rangle$. That is, each basis state represented in $|\xi\rangle$ must have the same number p of qubits in the state $|1\rangle$. (ii) $|\xi\rangle$ has no component in which two neighboring qubits are both in the state $|1\rangle$. (iii) The nth qubit is in the state $|0\rangle$. (This last condition effectively extends condition (ii) to the boundary between successive blocks.) Condition (i) guarantees that the density matrix ρ for a pair of nearest neighbors is block diagonal, each block corresponding to a fixed number of 1's in the pair. That is, there are two single-element blocks corresponding to $|00\rangle$ and $|11\rangle$, and a 2x2 block corresponding to $|01\rangle$ and $|10\rangle$. Conditions (ii) and (iii) guarantee that ρ_{44} is zero. The conditions thus give us the form (2.1). We impose these three conditions because they seem likely to give the best results; we do not prove that they are optimal.

To illustrate the three conditions and how they can be used, let us consider in detail the case where the block size n is 5 and the number p of 1's in each block is 2. (Our strategy does not specify the value of either n or p; these values will ultimately have to be determined by explicit maximization.) In this case, the only basis states our conditions allow in the construction of $|\xi\rangle$ are $|10100\rangle$, $|10010\rangle$, and $|01010\rangle$. Any other basis state either would have a different number of 1's or would violate one of conditions (ii) and (iii). Thus we write

$$|\xi\rangle = a_{13}|10100\rangle + a_{14}|10010\rangle + a_{24}|01010\rangle. \tag{2.3}$$

The subscripts in a_{ij} indicate which qubits are in the state $|1\rangle$. The state w of the infinite string is derived from $|\xi\rangle$ as described above. We now want to use Eq. (2.3) to write the density matrix ρ of a pair of nearest neighbors when the infinite string is in the state w. For definiteness let us take the two qubits of interest to be in locations $j = 1$ and $j = 2$, and let us take the 5-qubit blocks in the state w_0 to be given by $j = 1, \ldots, 5$, $j = 6, \ldots, 10$, and so on. Our final density matrix ρ will be an equal mixture of five density matrices, corresponding to the five different displacements of w_0 (including the null displacement).

For w_0 itself, the qubits at $j = 1$ and $j = 2$ are the first two qubits of $|\xi\rangle$. The density matrix for these two qubits, obtained by tracing out the other three qubits of the block, is

$$\rho^{(0)} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & |a_{24}|^2 & \overline{a}_{14}a_{24} & 0 \\ 0 & a_{14}\overline{a}_{24} & |a_{13}|^2 + |a_{14}|^2 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}. \tag{2.4}$$

For w_1, the qubits at $j = 1$ and $j = 2$ are now the second and third qubits of the block, since the block has been shifted to the left. Thus we trace over the first, fourth, and fifth qubits to obtain

$$\rho^{(1)} = \begin{pmatrix} |a_{14}|^2 & 0 & 0 & 0 \\ 0 & |a_{13}|^2 & 0 & 0 \\ 0 & 0 & |a_{24}|^2 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}. \tag{2.5}$$

In a similar way one can find $\rho^{(2)}$ and $\rho^{(3)}$:

$$\rho^{(2)} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & |a_{14}|^2 + |a_{24}|^2 & \overline{a}_{13}a_{14} & 0 \\ 0 & a_{13}\overline{a}_{14} & |a_{13}|^2 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}; \rho^{(3)} = \begin{pmatrix} |a_{13}|^2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & |a_{14}|^2 + |a_{24}|^2 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}.$$

The density matrix corresponding to w_4 is different in that the two relevant qubits now come from different blocks: the qubit at $j = 1$ is the last qubit of one block and the qubit at $j = 2$ is the first qubit of the next block. The corresponding density matrix is thus the tensor product of two single-qubit states:

$$\rho^{(4)} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \otimes \begin{pmatrix} |a_{24}|^2 & 0 \\ 0 & |a_{13}|^2 + |a_{14}|^2 \end{pmatrix} = \begin{pmatrix} |a_{24}|^2 & 0 & 0 & 0 \\ 0 & |a_{13}|^2 + |a_{14}|^2 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}.$$

To get the neighboring-pair density matrix corresponding to our final state w, we average the above five density matrices, with the following simple result:

$$\rho = \frac{1}{5} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 2 & x & 0 \\ 0 & \overline{x} & 2 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \tag{2.6}$$

where

$$x = \overline{a}_{13} a_{14} + \overline{a}_{14} a_{24}. \tag{2.7}$$

According to Eq. (2.2), the concurrence of the pair is

$$C = \frac{2}{5} \left| \overline{a}_{13} a_{14} + \overline{a}_{14} a_{24} \right|. \tag{2.8}$$

Continuing with this example—$n = 5$ and $p = 2$—let us find out what values we should choose for a_{13}, a_{14}, and a_{24} in order to maximize C. First, it is clear that we cannot go wrong by taking each a_{ij} to be real and non-negative—any complex phases could only reduce the absolute value in Eq. (2.8)—so let us restrict our attention to such values. To take into account the normalization condition, we use a Lagrange multiplier $\gamma/2$ and extremize the quantity

$$a_{13} a_{14} + a_{14} a_{24} - (\gamma/2)(a_{13}^2 + a_{14}^2 + a_{24}^2). \tag{2.9}$$

Differentiating, we arrive at three linear equations expressed by the matrix equation

$$\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} a_{13} \\ a_{14} \\ a_{24} \end{pmatrix} = \gamma \begin{pmatrix} a_{13} \\ a_{14} \\ a_{24} \end{pmatrix}. \tag{2.10}$$

Of the three eigenvalues, only one allows an eigenvector with non-negative components, namely, $\gamma = \sqrt{2}$. The normalized eigenvector is

$$\begin{pmatrix} a_{13} \\ a_{14} \\ a_{24} \end{pmatrix} = \begin{pmatrix} \frac{1}{2} \\ \frac{1}{\sqrt{2}} \\ \frac{1}{2} \end{pmatrix}, \tag{2.11}$$

which gives $C = \sqrt{2}/5 = 0.283$. This is greater than the value 0.25 that we obtained in our earlier example.

Before generalizing this calculation to arbitrary values of n and p, we adopt some terminology that will simplify the discussion. Let us think of the qubits as "sites," and let us call the two states of each qubit "occupied" ($|1\rangle$) and "unoccupied" ($|0\rangle$). The states $|\xi\rangle$ that we are considering have a fixed number p of occupied sites in a string of n sites; so we can regard the system as a collection of p "particles" in a one-dimensional lattice of length n. Condition (ii) requires that two particles never be in adjacent sites; it is as if each particle is an extended object, taking up two lattice sites, and two particles cannot overlap. Thus the number of particles is limited by the inequality $2p \leq n$.

3. Generalization to blocks of arbitrary size

We now turn to the calculation of the optimal concurrence for general n and p assuming our conditions are satisfied. It will turn out that this calculation can be done exactly.

For any values of n and p, the most general form of $|\xi\rangle$ consistent with condition (i) is

$$|\xi\rangle = \sum_{j_1<\cdots<j_p} a_{j_1,\ldots,j_p}|j_1,\ldots,j_p\rangle, \tag{3.1}$$

where $|j_1,\ldots,j_p\rangle$ is the state of n sites $j = 1,\ldots,n$ in which sites $j_1,\ldots,j_p$ are occupied and the rest are unoccupied. Because of conditions (ii) and (iii), $a_{j_1,\ldots,j_p}$ must be zero if two of the indices differ by 1 or if j_p has the value n. The coefficients in Eq. (3.1) satisfy the normalization condition

$$\sum_{j_1<\cdots<j_p} |a_{j_1,\ldots,j_p}|^2 = 1. \tag{3.2}$$

Going through the same steps as in the above example, we find that in the state w the density matrix of any pair of neighboring sites is

$$\rho = \frac{1}{n}\begin{pmatrix} n-2p & 0 & 0 & 0 \\ 0 & p & y & 0 \\ 0 & \overline{y} & p & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \tag{3.3}$$

where

$$y = \sum_{q=1}^{p}\sum_{j_1<\cdots<j_p}\sum_{j_1'<\cdots<j_p'}\left[\overline{a}_{j_1,\ldots,j_p}a_{j_1',\ldots,j_p'}\delta_{j_q',j_q+1}\prod_{r\neq q}\delta_{j_r',j_r}\right]. \tag{3.4}$$

Here δ is the Kronecker delta, and we define $a_{j_1,\ldots,j_p}$ to be zero if any two of the indices are equal. In words, y is constructed as follows: Let two coefficients $a_{j_1,\ldots,j_p}$ and $a_{j_1',\ldots,j_p'}$ be called adjacent if they differ in only one index and if the difference in that index is exactly one; then y is the sum of all products of adjacent pairs of coefficients, the coefficient with the smaller value of the special index being complex conjugated in each case. In the above example there were only two such products, $\overline{a}_{13}a_{14}$ and $\overline{a}_{14}a_{24}$; hence the form of Eq. (2.7).

As before, the concurrence of the chain is equal to $2|\rho_{23}|$; that is, $C = (2/n)|y|$. We want to maximize the concurrence over all possible values of the coefficients that are consistent with conditions (ii) and (iii). These conditions are somewhat awkward to enforce directly: one has to make sure that certain of the coefficients $a_{j_1,\ldots,j_p}$ are zero. However, this problem is easily circumvented by defining a new set of indices. Let $k_1 = j_1$, $k_2 = j_2-1$, $k_3 = j_3-2$, and so on up to $k_p = j_p-(p-1)$, and let $b_{k_1,\ldots,k_p} = a_{j_1,\ldots,j_p}$. The constraints on the new indices k_r are simply that $0 < k_1 < k_2 < \cdots < k_p < n'$, where $n' = n-(p-1)$. Finally, in place of $|\xi\rangle$, define a new vector $|\zeta\rangle$:

$$|\zeta\rangle = \sum_{k_1<\cdots<k_p} b_{k_1,\ldots,k_p}|k_1,\ldots,k_p\rangle, \tag{3.5}$$

where $|k_1,\ldots,k_p\rangle$ is the state of a lattice of length $n'-1$ in which the sites $k_1,\ldots,k_p$ are occupied. In effect we have removed from the lattice the site lying to the right of each occupied site. Note that our earlier inequality $2p \leq n$ becomes, in terms of

n', simply $p \leq n'-1$, which reflects the fact that the new lattice has only $n'-1$ sites. The concurrence is still given by $C = (2/n)|y|$, where

$$y = \sum_{q=1}^{p} \sum_{k_1 < \cdots < k_p} \sum_{k'_1 < \cdots < k'_p} \left[\overline{b}_{k_1,\ldots,k_p} b_{k'_1,\ldots,k'_p} \delta_{k'_q,k_q+1} \prod_{r \neq q} \delta_{k'_r,k_r} \right]. \tag{3.6}$$

We can express y more simply by introducing creation and annihilation operators for each site. We associate with site k the operators

$$c_k = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \text{ and } c_k^\dagger = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, \tag{3.7}$$

which are represented here in the basis $\{|0\rangle, |1\rangle\}$. In terms of these operators, we can write y as

$$y = \langle \zeta | \sum_{k=1}^{n'-2} c_k^\dagger c_{k+1} | \zeta \rangle. \tag{3.8}$$

Our problem is beginning to resemble the nearest-neighbor tight-binding model for electrons in a one-dimensional lattice. The Hamiltonian for the latter problem—assuming that the spins of the electrons are all in the same state and can therefore be ignored—can be written as[3]

$$H = -\sum_{k=1}^{n'-2} (c_k^\dagger c_{k+1} + c_{k+1}^\dagger c_k), \tag{3.9}$$

where we have taken the lattice length to be the same as in our problem, namely, $n'-1$. From Eqs. (3.8) and (3.9) we see that $\langle \zeta | H | \zeta \rangle = -2\,\mathrm{Re}(y)$. This expectation value is not quite what we need for the concurrence: the concurrence is proportional to the absolute value of y, not its real part. However, as in our earlier example, for the purpose of maximizing C there is no advantage in straying from real, non-negative values of $b_{k_1,\ldots,k_p}$. If we restrict our attention to such values, then the absolute value of y is the same as its real part, and we can write the concurrence as

$$C = -\frac{1}{n} \langle \zeta | H | \zeta \rangle. \tag{3.10}$$

Thus, maximizing the concurrence amounts to minimizing the expectation value of H, that is, finding the ground state energy of the tight-binding model, as long as the ground state involves only real and non-negative values of $b_{k_1,\ldots,k_p}$.

The one-dimensional tight-binding model is in fact easy to solve [**16, 17**]. Its ground state is the discrete analogue of the ground state of a collection of p non-interacting fermions in a one-dimensional box. In our case the "walls" of the box, where the wavefunction goes to zero, are at $k = 0$ and $k = n'$, and the ground state $|\zeta_0\rangle$ is given by the following antisymmetrized product of sine waves:

$$b_{k_1,\ldots,k_p} \propto \mathcal{A}\Big[\sin\Big(\frac{\pi k_p}{n'}\Big) \sin\Big(\frac{2\pi k_{p-1}}{n'}\Big) \cdots \sin\Big(\frac{p\pi k_1}{n'}\Big) \Big]. \tag{3.11}$$

[3]In Eq. (3.9) the operators c and $c^\dagger$ are fermionic, whereas those defined in Eq. (3.7) are not, because they do not anticommute when they are associated with different sites. We could, however, use our c's to define genuinely fermionic operators in terms of which the extremization problem has exactly the same form [**16**].

Here $\mathcal{A}$ indicates the operation of antisymmetrizing over the indices $k_1, \ldots, k_p$. In the range of values we are allowing for these indices, that is, $0 < k_1 < k_2 < \cdots < k_p < n'$, the coefficients $b_{k_1,\ldots,k_p}$ are indeed non-negative, so that Eq. (3.10) is valid.

The ground state energy, from which we can find the concurrence, is simply the sum of the first p single-particle eigenvalues of H. There are exactly $n' - 1$ such eigenvalues, one for each dimension of the single-particle subspace; they are given by

$$E_m = -2\cos\left(\frac{m\pi}{n'}\right), \; m = 1, \ldots, n'-1. \tag{3.12}$$

Thus the concurrence is

$$C = -\frac{1}{n}\langle\zeta_0|H|\zeta_0\rangle = \frac{2}{n}\sum_{m=1}^{p}\cos\left(\frac{m\pi}{n'}\right). \tag{3.13}$$

Doing the sum is straightforward, with the following result:

$$C = \frac{1}{n}\left[\frac{\cos(p\pi/n') - \cos((p+1)\pi/n') + \cos(\pi/n') - 1}{1 - \cos(\pi/n')}\right]. \tag{3.14}$$

Recall that $n' = n - p + 1$. Eq. (3.14) gives the largest value of C consistent with our conditions, for fixed values of n and p. Note, for example, that when $n = 5$ and $p = 2$, Eq. (3.14) gives $C = \sqrt{2}/5$, just as we found before for this case.

We still need to optimize over n and p. It is best to make the block size n very large—any state w that is possible with block size n is also allowed by block size $2n$—so we take the limit as n goes to infinity. Let α be the density of occupied sites—that is, $\alpha = p/n$—and let n approach infinity with α held fixed. In this limit, the concurrence becomes

$$C_{\text{lim}} = \frac{2}{\pi}(1-\alpha)\sin\left(\frac{\alpha\pi}{1-\alpha}\right). \tag{3.15}$$

Taking the derivative, one finds that C_{lim} is maximized when

$$\tan\left(\frac{\alpha\pi}{1-\alpha}\right) = \frac{\pi}{1-\alpha}, \tag{3.16}$$

which happens at $\alpha = 0.300844$, where $C_{\text{lim}} = 0.434467$. This is the highest value of concurrence that is consistent with our method of constructing the state of the chain and with our three conditions on $|\xi\rangle$. Note that it is considerably larger than what we got in our first example, in which a string of singlets was mixed with a shifted version of the same string—one might call this earlier construction the "bicycle chain" state. Unlike the bicycle chain state, our best state breaks the symmetry between the basis states $|0\rangle$ and $|1\rangle$: the fraction of qubits in the state $|1\rangle$ is about 30% rather than 50%. Of course the entanglement would be just as large if the roles of $|1\rangle$ and $|0\rangle$ were reversed.

It is interesting to ask what value of entanglement of formation the above value of concurrence corresponds to. As a function of the concurrence, the entanglement of formation is given by

$$E_f = h\left(\frac{1+\sqrt{1-C^2}}{2}\right), \tag{3.17}$$

where h is the binary entropy function $h(x) = -[x\log_2 x + (1-x)\log_2(1-x)]$. For the above value of concurrence, one finds that the entanglement of formation is $E_f = 0.284934$ ebits. (For the bicycle chain state, the entanglement of formation between neighboring pairs is only 0.118 ebits.)

If one can prove that this value is optimal, then it can serve as a reference point for interpreting entanglement values obtained for real physical systems. A string of spin-1/2 particles interacting via the antiferromagnetic Heisenberg interaction, for example, has eigenstates that typically have some non-zero nearest-neighbor entanglement. It would be interesting to find out how the entanglements appearing in these states compare to the maximum possible entanglement for a string of qubits.[4]

Clearly the problem we have analyzed here can be generalized. One can consider a two or three-dimensional lattice of qubits and ask how entangled the neighboring qubits can be. If we were to analyze these cases using assumptions similar to those we have made in the one-dimensional case, we would again find the problem reducing to a many-body problem, but with less tractable interactions. Assuming that pairwise entanglement tends to diminish as the total entanglement is shared among more particles, one expects the optimal values of C and E_f to shrink as the dimension of the lattice increases.

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[4] Since the original version of this paper was written, the question about the antiferromagnetic Heisenberg chain has been answered for the ground state [**18**]: though the nearest-neighbor concurrence of the ground state is high ($C = 0.386$), it is not optimal.

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