Infinite qubit rings with maximal nearest-neighbor entanglement: The Bethe ansatz solution

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We search for translationally invariant states of qubits on a ring that maximize the nearest-neighbor entanglement. This problem was initially studied by O'Connor and Wootters [Phys. Rev. A **63**, 052302 (2001)]. We first map the problem to the search for the ground state of a spin-1/2 Heisenberg *XXZ* model. Using the exact Bethe ansatz solution in the limit $N\to\infty$, we prove the correctness of the assumption of O'Connor and Wootters that the state of maximal entanglement does not have any pair of neighboring spins "down" (or, alternatively, spins "up"). For sufficiently small fixed magnetization, however, the assumption does not hold: we identify the region of magnetizations for which the states that maximize the nearest-neighbor entanglement necessarily contain pairs of neighboring spins "down."

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I. INTRODUCTION

The investigation of the role of entanglement in quantum and classical phase transitions, and more generally the role of entanglement in many-body quantum systems, is one of the hottest interdisciplinary areas on the borders between quantum information, quantum optics, atomic, molecular, and condensed matter physics. Initially the studies of entanglement in many-body systems have been motivated by the possibility of employing entanglement for quantum computation in optical lattices [1] or precision measurements with Bose-Einstein condensates [2]. Recently, several lines of research have been followed.

(i) Studies of local entanglement in spin systems [3–7], and more generally in various many-body systems (such as linear chains, see, for instance, [8–10]), with particular attention to the role of entanglement in phase transitions.

(ii) Studies of the entropy of blocks of spins and the related "area law" [11], indicating weak entanglement of blocks, and effects of criticality [5,12,10,13].

(iii) Studies of localizable entanglement and entanglement correlation length that diverges at the critical point [14,15] and majorizes the standard correlation length (see also [16]). In particular, it has been shown that the localizable entanglement (cf. [17–19]) is bounded from above by the entanglement of assistance [20] and from below by correlation functions. It follows directly from these bounds that one can define an entanglement correlation length that diverges in quantum critical systems.

(iv) Studies of multipartite entanglement in many-body systems [21].

(v) Studies of dynamics and generation of entanglement in many-body systems [13,22–25]. In particular, implementations of the "one-way quantum computer" and short-range teleportation [26] of an unknown state has been proposed by using the dynamics of spin systems in Refs. [13,22,25,27–29].

(vi) Studies of quantum information and entanglement theory inspired numerical codes to simulate quantum systems [30].

A different approach to the study of entanglement in many-body systems has been proposed in two papers by Wootters and O'Connor [31]. In these papers, instead of looking at a specific Hamiltonian, the authors asked the fundamental question, what is the maximal entanglement between two neighboring sites of an entangled ring with translational invariance? Here, an entangled ring is a chain of spins 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 [32,33]. In Ref. [31] the question of the upper limit for the nearest-neighbor (NN) entanglement was simplified by introducing two additional restrictions on the allowed states.

(i) The state of N spins 1/2 is an eigenstate of the z component of the total spin (i.e., it has a fixed number of "down" spins $p\leqslant N/2$).[1]

(ii) Neighboring spins cannot both be "down."

Obviously, one can equally well study the same problem in terms of spins "up" when $N\geqslant p\geqslant N/2$. Both restrictions are based on an educated guess for the optimal states for the general problem. O'Connor and Wootters (OW) 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 (cf. Sec. II) for a given N and p to be

$$C_{\mathrm{OW}}^{\max}(N,p)=\frac{2\sin\left(\frac{p\pi}{N-p}\right)}{N\sin\left(\frac{\pi}{N-p}\right)}. \tag{1}$$

For given N and p, Eq. (1) provides a lower bound for the problem without restriction (ii). It may or may not happen

[1]Note that one can also allow the state to be an incoherent mixture of several states, each with a fixed p: Since we will be optimizing a convex function, such a mixture cannot be optimal. Thus restriction (i) can be replaced with the formally weaker demand that the density operator commutes with the z component of the total spin [34].

that C can be increased by also allowing states where two neighboring spins are "down." We have recently studied finite-size rings and found that for a fixed p restriction (ii) tends to play a less important role as N is increased [34]: For p close to $N/2$ one can increase the concurrence significantly by dropping restriction (ii), but for $p \lesssim N/3$ OW's result is the optimal one. In fact, already in Ref. [31] it was shown that for all even N the ground state of a Heisenberg spin-1/2 antiferromagnetic ring maximizes the concurrence among the zero magnetization ($p=N/2$) states although it violates restriction (ii).

By optimizing Eq. (1) with respect to p one obtains a lower bound on the overall optimal concurrence—i.e., without any restrictions besides the translational invariance. In the limit $N\to\infty$, the optimal number of spins "down" in Eq. (1) approaches $p_{\mathrm{opt}}\approx 0.301N$. This leads to an asymptotic value of $C_{\mathrm{OW}}^{\max}\approx 0.434$. Although Ref. [31] as well as our previous work [34] and the recent work by Hiesmayr *et al.* [35] all showed evidence for the optimality of this number, whether it can be improved has, so far, been an open problem.

Wolf, Verstraete, and Cirac have in Ref. [36] directly related OW's type of problems of looking for translationally invariant states that maximize local entanglement to the study of the ground state of a suitably defined "parent" Hamiltonian. In this paper we use this method and employ the known exact solution of the corresponding parent Hamiltonian to prove rigorously the following.

(A) In the limit $N\to\infty$ the translationally invariant state that maximizes the NN entanglement without any restriction coincides with the state found by OW at the optimal value of $p\simeq 0.301N$. This means that it is not a superposition of states with different p values and does not contain simultaneously neighboring spin-"up" and neighboring spin-"down" pairs.

(B) For fixed p sufficiently close to $N/2$—i.e., for sufficiently small magnetizations—assumption (ii) is not correct: the states that maximize the nearest-neighbor entanglement necessarily contain simultaneously pairs of neighboring "up" and "down" spins. In the limit $N\to\infty$ we identify rigorously an interval of p/N for which this is the case and show strong numerical evidence that this interval is optimal.

Our paper is organized as follows. In Sec. II we apply the method of Ref. [36] and derive the corresponding parent Hamiltonian for an N-qubit ring. In Sec. III we show the connection with the "classical" papers of Yang and Yang on the XXZ model. In Sec. IV we discuss briefly the regimes of parameters of interest and show that the present problem concerns the "difficult" parameter region of the phase diagram. In Sec. V we present an analysis based on the limit $N\to\infty$ of the Bethe ansatz solutions. We derive here the basic integral equation, the solution of which allows us to calculate the desired energy of the system in question. In Sec. VI the numerical results are discussed. In Sec. VII we rigorously prove that the states that were conjectured in Ref. [31] to maximize the NN entanglement and confirmed by us indeed provide the maximum of the NN entanglement for sufficiently small values of p. We identify the region of p/N where the latter statement does not hold. We conclude in Sec. VIII. The short appendix contains simple analytic bounds on optimal magnetic field for which the NN concurrence is maximal.

II. VARIATIONAL CONCURRENCE FORMULA

In this paper we will use the concurrence as our entanglement measure. The concurrence [37] is defined as $C(\rho)=\max\{\lambda_1-\lambda_2-\lambda_3-\lambda_4,0\}$, where $\lambda_1\geq\lambda_2\geq\lambda_3\geq\lambda_4\geq 0$ are the square roots of the eigenvalues of $\rho\tilde{\rho}$ and $\tilde{\rho}=(\sigma_y\otimes\sigma_y)\rho^*(\sigma_y\otimes\sigma_y)$ is the spin-flipped density matrix. The optimization problems that we consider are complicated by the nonlinearity of the concurrence as function of the density matrix. In our previous work [34], we showed how the optimization problem with fixed p can be reformulated as finding the ground-state energy for each in a family of spin-chain Hamiltonians. This family is parametrized by a single real parameter, and the optimal concurrence is minus the lowest ground-state energy that occurs when this parameter is varied. In this way a complicated nonlinear problem in a high-dimensional space is replaced by a series of linear problems and one final one-parameter optimization.

The derivation in Ref. [34] did not cover the case where superpositions of states with different p are allowed. To treat that case, we turn to Ref. [36] where the following general formula for the concurrence for systems of two spins 1/2 has been derived:

$$C(\rho)=\max\left\{0,-\inf_{\det X=1}\mathrm{tr}[\rho(X\otimes X^\dagger)\mathbf{F}]\right\}. \tag{2}$$

Here X is an arbitrary 2×2 matrix of determinant 1, while $\mathbf{F}$ is the flip (or swap) operator, interchanging the two qubits:

$$\mathbf{F}=|\uparrow\uparrow\rangle\langle\uparrow\uparrow|+|\downarrow\downarrow\rangle\langle\downarrow\downarrow|+|\downarrow\uparrow\rangle\langle\uparrow\downarrow|+|\uparrow\downarrow\rangle\langle\downarrow\uparrow|. \tag{3}$$

A useful parametrization of X is obtained using the singular value decomposition [38]

$$X=U\begin{bmatrix} it & 0\\ 0 & \dfrac{1}{it}\end{bmatrix}V^\dagger, \tag{4}$$

where $t\in[-\infty,\infty]$, $U,V\in\mathrm{U}(2)$ and $\det U\det V^\dagger=1$. In fact, from Eq. (2) it is clear that we can restrict ourselves to $U,V\in\mathrm{SU}(2)$. We now rewrite

$$\begin{aligned} X\otimes X^\dagger\mathbf{F}&=(U\otimes V)\left(\begin{bmatrix} it & 0\\ 0 & \dfrac{1}{it}\end{bmatrix}\otimes\begin{bmatrix} -it & 0\\ 0 & \dfrac{1}{-it}\end{bmatrix}\right)(V^\dagger\otimes U^\dagger)\mathbf{F}\\ &=(U\otimes V)\begin{bmatrix} t^2 & 0 & 0 & 0\\ 0 & -1 & 0 & 0\\ 0 & 0 & -1 & 0\\ 0 & 0 & 0 & t^{-2}\end{bmatrix}\mathbf{F}(U\otimes V)^\dagger\\ &=(U\otimes V)\begin{bmatrix} t^2 & 0 & 0 & 0\\ 0 & 0 & -1 & 0\\ 0 & -1 & 0 & 0\\ 0 & 0 & 0 & t^{-2}\end{bmatrix}(U\otimes V)^\dagger. \end{aligned} \tag{5}$$

Let us define the matrix in square brackets as $h(t^2)$—i.e.,

$$h(s) = s|\uparrow\uparrow\rangle\langle\uparrow\uparrow| + \frac{1}{s}|\downarrow\downarrow\rangle\langle\downarrow\downarrow| - |\downarrow\uparrow\rangle\langle\uparrow\downarrow| - |\uparrow\downarrow\rangle\langle\downarrow\uparrow|, \tag{6}$$

where $s=t^2$. Then we can rewrite Eq. (2) as

$$C(\rho) = \max\left\{0, -\inf_{s,U,V} \mathrm{tr}[(U\otimes V)^\dagger \rho (U\otimes V) h(s)]\right\}. \tag{7}$$

Our goal is to maximize the concurrence over all ρ that can occur as nearest-neighbor density matrices on a translationally invariant ring. If we always had $U=V$, it is easy to see that we could drop the infimum over $U\in \mathrm{SU}(2)$ in Eq. (7) since if $\rho=\mathrm{tr}_{3,\ldots,N}\Gamma$ with Γ translationally invariant, then $(U\otimes U)^\dagger \rho (U\otimes U) = \mathrm{tr}_{3,\ldots,N}(U\otimes\cdots\otimes U)^\dagger \Gamma (U\otimes\cdots\otimes U)$ where $(U\otimes\cdots\otimes U)^\dagger\Gamma(U\otimes\cdots\otimes U)$ is translationally invariant as well. To do the same for $U\neq V$, we can use the fact that $h(s)$ is symmetric in the two qubits:

$$\mathrm{tr}[(U\otimes V)^\dagger \rho (U\otimes V) h(s)] = \mathrm{tr}[\tilde{\rho} h(s)], \tag{8}$$

where

$$\tilde{\rho} = \frac{1}{2}\{(U\otimes V)^\dagger \rho (U\otimes V) + (V\otimes U)^\dagger \rho (V\otimes U)\}. \tag{9}$$

If N is even and $\rho=\mathrm{tr}_{3,\ldots,N}\Gamma$, then $\tilde{\rho}$ is a nearest-neighbor density matrix belonging to the following translationally invariant state:

$$\begin{aligned}\frac{1}{2}\{&([U\otimes V]\otimes\cdots\otimes[U\otimes V])^\dagger \\ &\times\Gamma\times([U\otimes V]\otimes\cdots\otimes[U\otimes V]) \\ &+([V\otimes U]\otimes\cdots\otimes[V\otimes U])^\dagger \\ &\times\Gamma\times([V\otimes U]\otimes\cdots\otimes[V\otimes U])\}.\end{aligned} \tag{10}$$

If N is odd, the above construction does not work: we cannot fit an integer number of $U\otimes V$ terms on the ring. By placing as many terms $U\otimes V$ as possible and taking the translationally variant mixture of the resulting state, $\tilde{\rho}$ can be approximated up to a factor of $1/N$. In the limit of $N\to\infty$ we can ignore this correction.

III. PARENT HAMILTONIAN

In this section we will follow the approach of Ref. [36] to derive the parent spin-1/2 *XXZ* Hamiltonian—i.e., the Hamiltonian whose ground state maximizes the NN concurrence. We also make the connection to the classical papers on the *XXZ* model by Yang and Yang [39–41].

In the previous section we showed that, in the limit $N\to\infty$,

$$C^{\max}(N) = \max_\rho C(\rho) = -\inf_{s,\rho} \mathrm{tr}[\rho h(s)], \tag{11}$$

where $\rho=\mathrm{tr}_{3,\ldots,N}\Gamma$ for some translationally invariant Γ of N spins. The two-spin Hamiltonian (6) can be written in terms of Pauli matrices as

$$\begin{aligned}h(s) &= \frac{s}{4}(\mathbf{1}+\sigma_z)(\mathbf{1}+\sigma_z) + \frac{1}{4s}(\mathbf{1}-\sigma_z)(\mathbf{1}-\sigma_z) - \sigma_-\sigma_+ - \sigma_+\sigma_- \\ &= \frac{1}{2}\left\{-\sigma_x\sigma_x - \sigma_y\sigma_y + \frac{1}{2}\left(s+\frac{1}{s}\right)(\sigma_z\sigma_z+1) \right. \\ &\quad \left. + \frac{1}{2}\left(s-\frac{1}{s}\right)(\sigma_z\mathbf{1}+\mathbf{1}\sigma_z)\right\},\end{aligned} \tag{12}$$

where $\sigma_\pm=\sigma_x\pm i\sigma_y$. Instead of working with ρ and $h(s)$ we can use the translational invariance and work with Γ and a Hamiltonian for the whole ring obtained by taking Eq. (12) for each NN pair:

$$\begin{aligned}H_{\mathrm{Wolf}}(s) = \frac{1}{2N}\sum_{i=1}^{N}\{&-\sigma_x^i\sigma_x^{i+1} - \sigma_y^i\sigma_y^{i+1} - \Delta(s)\sigma_z^i\sigma_z^{i+1} \\ &- 2\mathcal{H}(s)\sigma_z^i - \Delta(s)\},\end{aligned} \tag{13}$$

where

$$\Delta(s) = -\frac{1}{2}\left(s+\frac{1}{s}\right), \quad \mathcal{H}(s) = -\frac{1}{2}\left(s-\frac{1}{s}\right). \tag{14}$$

We have then reformulated the overall optimization problem as

$$C^{\max}(N) = \max_\rho C(\rho) = -\inf_{s,\Gamma} \mathrm{tr}[\Gamma H_{\mathrm{Wolf}}(s)], \tag{15}$$

where ρ is restricted to arise from a translationally invariant state of N spins while the optimal Γ can automatically be chosen so since H_{Wolf} is translationally invariant.

An important observation can be made from Eq. (15)—namely, that as H_{Wolf} commutes with the z component of the total spin, in the considered limit of $N\to\infty$, OW were right when they made assumption (i): The optimal state can indeed be chosen to have a definite number of spins "down" and thus does not contain superpositions of states with different p values. Conversely, from our previous work [34] we know that Eq. (15) is also valid for any fixed p; i.e., we can write $C^{\max}(N,p)$ on the left-hand side when making the appropriate restrictions on Γ. In summary, for fixed p the maximal concurrence is given by

$$C^{\max}(N,p) = -\inf_s E_{\mathrm{GS}}[H_{\mathrm{Wolf}}(s),p], \tag{16}$$

where $E_{\mathrm{GS}}[H_{\mathrm{Wolf}}(s),p]$ is the "ground-state" energy of $H_{\mathrm{Wolf}}(s)$ in the manifold of states with p spins "down." The overall maximal concurrence is given by further optimization over p or, equivalently, by using unrestricted ground-state energies:

$$C^{\max}(N) = \max_p C^{\max}(N,p) = -\inf_s E_{\mathrm{GS}}[H_{\mathrm{Wolf}}(s)]. \tag{17}$$

Let us now describe the connection with the work of Yang and Yang. In their seminal papers Yang and Yang [39–41] study this anisotropic Heisenberg *XXZ* Hamiltonian (see, e.g., [42] for more recent work)

$$H_{\mathrm{Yang}} = -\frac{1}{2}\sum_i \{\sigma_x^i\sigma_x^{i+1} + \sigma_y^i\sigma_y^{i+1} + \Delta\sigma_z^i\sigma_z^{i+1}\}, \quad (18)$$

and they define $f=\lim_{N\to\infty} f_N$, where f_N is half the energy per spin in the ground state with a given number p of spins "down":

$$f_N(\Delta, y) = \frac{1}{2N} E_{\mathrm{GS}}[H_{\mathrm{Yang}}, p]. \quad (19)$$

Here y is the average magnetization:

$$y = \frac{1}{N}\left\langle \sum_i \sigma_z^i \right\rangle = 1 - \frac{2p}{N}. \quad (20)$$

Since p is a conserved quantum number, one can include a magnetic field along z and only shift the energy of each eigenstate. The translation of the results of Yang and Yang to our optimization problems is, therefore,

$$E_{\mathrm{GS}}[H_{\mathrm{Wolf}}(s), p] = 2f_N(\Delta(s), y) - \mathcal{H}(s)y - \frac{1}{2}\Delta(s), \quad (21)$$

with $s>0$. Note that $\Delta^2-\mathcal{H}^2=1$. To find $C^{\max}(N,p)$ we should minimize Eq. (21) over s while keeping y fixed at the value corresponding to p [cf. Eq. (20)]. To find the overall maximal concurrence $C^{\max}(N)$ we should furthermore minimize over y.

IV. PHASE DIAGRAM OF THE *XXZ* MODEL

In Sec. III we found that we should consider infinite spin chains with *XXZ* interaction between neighboring spins and subject to a magnetic field. A slightly unusual feature is that we will sometimes keep the magnetization y fixed and search for the minimal energy state only inside the corresponding manifold [cf. Eq. (16)]. However, when we seek the overall optimal concurrence, we are in the normal situation where one views the magnetization as a function of the magnetic field. It is then useful to relate our problem to the phase diagram for the *XXZ* model, displayed in Fig. 1.

Let us first identify the region of the phase diagram which belongs to our parent Hamiltonian (13). From Eq. (14) it is clear that as s varies from 0 to ∞, we move on a hyperbola in the Δ-$\mathcal{H}$ plane: The $s=0$ case corresponds to $(-\infty,\infty)$, whereas at $s=1$ we are at the point of closest approach and cross the Δ axis in $(-1,0)$, and as $s\to\infty$ we move back to infinity, but this time with negative magnetic field. Comparing this with Fig. 1, it is then easy and not surprising to see that the s hyperbola lies exactly in the "difficult" region of the phase diagram—i.e., the part with neither perfectly aligned spins nor perfect antiferromagnetic order (between AF and A in Fig. 1).

Since a change of sign of the magnetic field will only interchange the role of spin "up" and spin "down," we can ignore the negative $\mathcal{H}$ branch and focus on $s\in[0,1]$. Then each point on the curve corresponds to exactly one Δ and we can thus parametrize the curve by Δ instead of s. The optimization is then done over Δ with the magnetic field always given by $\mathcal{H}=\sqrt{\Delta^2-1}$.

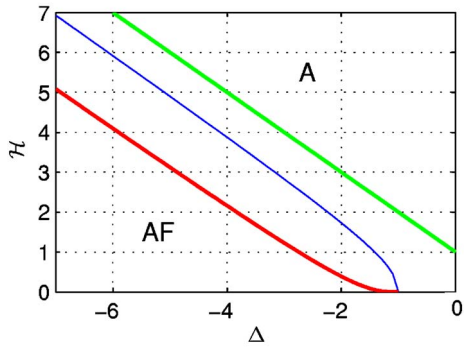

FIG. 1. (Color online) Phase diagram for the *XXZ* chain in a magnetic field [43]. For large negative Δ and small magnetic field $\mathcal{H}$ the ground state has perfect antiferromagnetic ordering (AF) with vanishing magnetization. When the magnetic field is increased beyond a certain critical value (lower bold line in the plot), a nonvanishing magnetization develops. The magnetization increases with increasing field until finally all the spins are aligned. This aligned phase (A) is entered at an upper critical field indicated by the upper thick line in the plot. We are interested in the properties of the chain along the thin line in the plot; i.e., we deal with the phase with nonvanishing, but also nonsaturated magnetization.

V. INTEGRAL EQUATION

The Bethe ansatz basically consists of the assumption that the wave function can be written as a sum of plane waves with a limited number of terms. If we are looking for a state with p spins "down," only p wave numbers are needed. For the case of the *XXZ* chain, the first Yang-Yang article shows that this is indeed enough to produce the ground-state wave function for any p [39]. In the limit of $N\to\infty$, the number of needed wave numbers naturally becomes infinite and the equation to find them becomes an integral equation for the wave number density. Instead of the number of spins "down" one fixes the fraction p/N and thus by Eq. (20) the magnetization y. The integral equation mathematically has the form of a so-called *Fredholm equation of the second kind*. After some reparametrization the equation to be solved attains the form [Eq. (7a) in Ref. [40]]

$$R(\alpha) = \frac{dp}{d\alpha} - \frac{1}{2\pi}\int_{-b}^{b} \frac{\partial\theta}{\partial\beta} R(\beta)\, d\beta. \quad (22)$$

The unknown function here is R, which is the reparametrized density of wave numbers and thus characterizes the state. The other functions depend parametrically on Δ, and in terms of the parameter $\lambda=\cosh^{-1}(-\Delta)$, they are explicitly given by

$$\frac{dp}{d\alpha} = \frac{\sinh\lambda}{\cosh\lambda - \cos\alpha}, \quad (23)$$

$$\frac{\partial\theta}{\partial\beta} = \frac{\sinh 2\lambda}{\cosh 2\lambda - \cos(\alpha-\beta)}. \quad (24)$$

The integration limit b in Eq. (22) is connected to the magnetization manifold we are considering: When varying b, we

get solutions corresponding to different values of y. The magnetization is found from

$$\pi(1-y) = \int_{-b}^{b} R(\alpha) d\alpha. \tag{25}$$

We emphasize that R depends on b, so the connection between b and y is not as direct as it may appear when only considering Eq. (25). In praxis (i.e., when doing numerics) one solves Eq. (22) for a range of values of the parameter b, calculates the corresponding y values from Eq. (25), and picks the solution resulting in the wanted value of y. If one wants to optimize some quantity with respect to y, however, this can equally well be achieved by optimizing with respect to b.

We are not primarily interested in R which describes the state. Rather we want f, which we then via Eq. (21) can use in Eq. (16). As for y, we need to do an integration to find f from R:

$$f(\Delta, y) = -\frac{\Delta}{4} - \frac{\sinh\lambda}{2\pi} \int_{-b}^{b} R(\alpha) \frac{dp}{d\alpha} d\alpha. \tag{26}$$

Again, f is written as a function of y, but in praxis the dependence is via b.

VI. NUMERICAL SOLUTION OF THE INTEGRAL EQUATION

A possible way to solve Eq. (22) is to turn the integral into a sum so that it becomes a matrix equation. This is called the *Nystrom method*.[2] The best way to discretize an integral is *not* always equally spaced points; very often it is much more efficient to use a *Gaussian quadrature*. This means that we evaluate the integrand at M points $\{\alpha_k\}$ and make a weighted sum with weights $\{w_k\}$. The points and the weights can be easily found in, e.g., *Mathematica*. In this way, Eq. (22) becomes:

$$R_k = \xi_k - \sum_l w_l K_{kl} R_l, \tag{27}$$

where

$$R_k = R(\alpha_k), \quad \xi_k = \frac{\sinh\lambda}{\cosh\lambda - \cos\alpha_k}, \tag{28}$$

while

$$K_{kl} = \frac{1}{2\pi} \frac{\sinh 2\lambda}{\cosh 2\lambda - \cos(\alpha_k - \alpha_l)}. \tag{29}$$

It is clear that Eq. (27) is a matrix equation and that solving it cannot be harder than inverting $\mathbf{1}+\tilde{K}$ where $\tilde{K}_{kl}=w_l K_{kl}$ (no summation over l).

The advantage of using Gaussian quadrature is that one does not need too many points to get a very good estimate of the integral for any sensible function. What exactly a "sensible function" is depends on the Gaussian quadrature rule used. We use the simple Gauss-Legendre rule, assuming that R is well approximated by a polynomial on the interval $[-b,b]$. This is reasonable here because Eqs. (23) and (24) are well behaved for the values of λ we will consider. The final matrix equation can be solved very rapidly on a small-size computer. A moderate value of M, however, means that our knowledge of R is restricted to a rather crude sampling; fortunately, this is not a problem, since y and f are themselves integrals and so can be evaluated with the full accuracy of Gaussian quadrature.

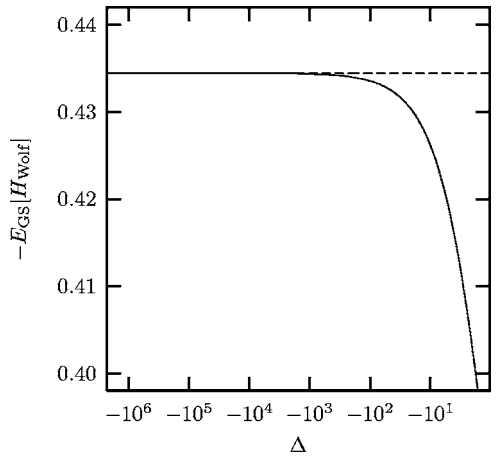

FIG. 2. We plot $-E_{GS}[H_{Wolf}]$; that is, for each Δ, the optimal y is chosen. It can be seen that the maximum is attained in the limit $\Delta \to -\infty$ and that the limiting value coincides with OW's result indicated by the dashed line.

To give the reader an idea about the numerics, we note that a simple *Mathematica* program will work very well with $M \leqslant 30$. Producing a plot of $f(\Delta, y)$ versus y for Δ not too close to -1 takes about 1 min. To plot the function of main interest, Eq. (21) optimized over p (i.e., y—i.e., b), also only takes a few minutes. In Fig. 2 we present the results of a FORTRAN program, which is (not surprisingly) much faster than the initial *Mathematica* code. The results indicate that OW's assumption (ii) was correct: When we plot $E_{GS}[H_{Wolf}]$ as function of Δ, we see that the optimal value of Δ is reached at $-\infty$, and in this limit OW's result is recovered. We conclude that these simple numerical results indicate that the state that maximizes the NN concurrence without any restrictions (i.e., optimized over p/N—i.e., y) coincides with the OW state fulfilling assumption (ii) (no NN pairs of spins "down").

VII. PERTURBATIVE CALCULATION

Looking at Eq. (21) above we see that the finite value in Fig. 2 in the limit $\Delta \to -\infty$ is obtained because some diverging terms happen to cancel each other. This is of course a great concern when doing numerics since it means that a good relative precision (knowing each term to, e.g., 1 ppm) may not be enough. The obvious strategy is to extract the solution in the strict limit $\Delta \to -\infty$. In this section, we will present a perturbative calculation in $1/\Delta$.

In zeroth order of the perturbation series we set $\cosh\lambda = \infty$ in Eq. (22) and arrive at the simple equation

[2] See, e.g., Numerical Recipes [44].

$$R_0(\alpha) = 1 - \frac{1}{2\pi}\int_{-b}^{b} R_0(\beta)d\beta. \tag{30}$$

The right-hand side does not depend on α, and we easily find the constant solution

$$R_0 = \frac{1}{1+b/\pi}, \quad y_0 = \frac{1-b/\pi}{1+b/\pi}. \tag{31}$$

This means that in this limit $f=-\Delta f_{-1}$ with

$$f_{-1} = \frac{1}{4} - \frac{b/\pi}{1+b/\pi} = -\frac{1}{4} + \frac{1}{2}y_0 \tag{32}$$

and that Eq. (21) thus gives 0, independently of y_0. At this level of precision we therefore get no information as to whether OW's solution is optimal for all y's.

The next order is "$1/\Delta$"; i.e., we expand both sides of Eq. (22) and equate terms proportional to $-1/\Delta = 1/\cosh\lambda$. We get

$$R_1(\alpha) = \cos\alpha - \frac{1}{2\pi}\int_{-b}^{b} R_1(\beta)d\beta. \tag{33}$$

The α dependence on the right-hand side (RHS) is $\cos\alpha$ plus a constant, so we easily find

$$R_1(\alpha) = \cos\alpha - \frac{\sin b}{\pi + b}, \quad y_1 = -\frac{2\sin b}{\pi + b}. \tag{34}$$

The correction to f is given by

$$f_0 = -\frac{1}{2\pi}\int_{-b}^{b}[-\cos\alpha R_0 + R_1(\alpha)]d\alpha = -\frac{2\sin b}{b+\pi} = y_1. \tag{35}$$

This means that in Eq. (21) we get a zeroth-order contribution of

$$E_{\mathrm{GS},0} = 2y_1 - y_1 = y_1 = -\frac{2\sin b}{b+\pi}. \tag{36}$$

It is easy to see that this expression is the same as the one obtained by OW in Ref. [31], and if we do a numerical optimization over b, we arrive at the notorious 0.434 467… for the maximal concurrence. This value is obtained for $b=b_{\mathrm{OW}}=1.351\,802\ldots$, corresponding by Eq. (25) to $y=y_{\mathrm{OW}}=0.398\,316\ldots$.

A. Recursion formula for higher-order corrections

It is tedious, but essentially not difficult to continue in the above fashion and calculate higher-order corrections. A useful trick is to develop a recursion formula. Let us write $\epsilon = 1/|\Delta|$ and define

$$R(\alpha) = \sum_k R_k(\alpha)\epsilon^k,$$

$$\frac{dp(\alpha)}{d\alpha} = \sum_k \frac{dp_k(\alpha)}{d\alpha}\epsilon^k,$$

$$\frac{\partial\theta(\alpha,\beta)}{\partial\beta} = \sum_k \frac{\partial\theta_k(\alpha,\beta)}{\partial\beta}\epsilon^k. \tag{37}$$

The kth-order terms of Eq. (22) give us

$$R_k(\alpha) = \frac{dp_k(\alpha)}{d\alpha} - \frac{1}{2\pi}\int_{-b}^{b}\sum_{j=0}^{k}\frac{\partial\theta_{k-j}(\alpha,\beta)}{\partial\beta}R_j(\beta)d\beta. \tag{38}$$

Using the fact that $\frac{\partial\theta_0}{\partial\beta}=1$ we collect terms containing R_k on the left-hand side:

$$\int_{-b}^{b}\left[\delta(\alpha-\beta) + \frac{1}{2\pi}\right]R_k(\beta)d\beta = \frac{p_k}{d\alpha} - \frac{1}{2\pi}\int_{-b}^{b}\sum_{j=0}^{k-1}\frac{\partial\theta_{k-j}(\alpha,\beta)}{\partial\beta}R_j(\beta)d\beta = q_k(\alpha), \tag{39}$$

where we have introduced $q_k(\alpha)$ as a shorthand notation for the RHS. The RHS depends only on the known functions $dp/d\alpha$ and $\partial\theta/\partial\beta$ and on R_j for $j<k$. The integral operator acting on R_k on the LHS of Eq. (39) can easily be inverted since it is built from the identity and a projection operator (onto a constant). We finally end up with the recursion formula

$$R_k(\alpha) = q_k(\alpha) - \frac{1}{2}\frac{1}{b+\pi}\int_{-b}^{b} q_k(\beta)d\beta. \tag{40}$$

In terms of R_k and the auxiliary function q_k, we have for y_k, $k>0$,

$$y_k = 2[R_k(\alpha) - q_k(\alpha)]. \tag{41}$$

Note that despite the appearance of α on the right-hand side, this relation does make sense since the form of Eq. (40) ensures us that only terms independent of α survive.

Using Eq. (40), it is fairly easy to show that

$$R_2(\alpha) = \cos^2\alpha - \frac{\sin b}{b+\pi}\cos\alpha - \frac{1}{2}\frac{\sin b}{b+\pi}\left(\cos b - \frac{\sin b}{b+\pi}\right) - \frac{1}{2} \tag{42}$$

and thus

$$y_2 = -\frac{\sin b}{b+\pi}\left(\cos b - \frac{\sin b}{b+\pi}\right). \tag{43}$$

Calculating the first-order contribution to the ground-state energy we find the expression

$$E_{\mathrm{GS},1}(b) = \frac{1}{2} - \frac{b}{\pi} - \frac{1}{\pi}\frac{\sin b}{b+\pi}[(b+2\pi)\cos b - 2\sin b]. \tag{44}$$

B. Derivative at fixed y

As mentioned above, $E_{\mathrm{GS},1}$ gives us access to whether OW's solution is at least a *local* minimum for a given y. In Eq. (44), $E_{\mathrm{GS},1}$ is expressed as a function of b, so in order to

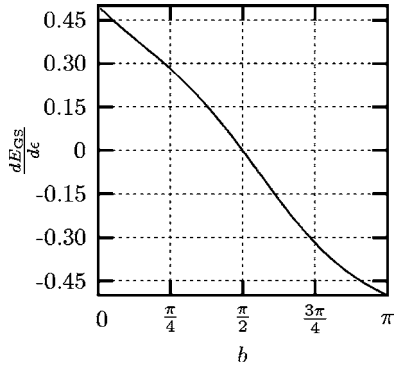

FIG. 3. Derivative of E_{GS} with respect to $\epsilon=1/|\Delta|$ for $\epsilon=0$ and fixed y. A positive value for a given b indicates that OW's solution is a local minimum for the corresponding y. Negative values indicate that OW's solution is not a local, and thus also not a global minimum.

calculate the derivative at fixed y we need to use the appropriate implicit differentiation rule. Calculating the lowest nonvanishing order we find

$$\left(\frac{dE_{GS}}{d\epsilon}\right)_y = \frac{\partial E_{GS}}{\partial \epsilon} + \frac{\partial E_{GS}}{\partial b}\left(\frac{\partial b}{\partial \epsilon}\right)_y$$
$$= E_{GS,1}(b) - \frac{dE_{GS,0}}{db}\frac{y_1}{dy_0/db} + O(\epsilon)$$
$$= \frac{1}{2} - \frac{b}{\pi} + \frac{b\sin b\cos b}{\pi(\pi+b)} + O(\epsilon). \qquad (45)$$

Again we end up with a somewhat complicated expression, so we plot its graph in Fig. 3. We note that $(dE_{GS}/d\epsilon)_y$ is positive for low b, but already at $b=\pi/2$ (corresponding to $y=1/3$) it changes sign and becomes negative. This means that for higher b's—i.e., lower y's—OW's solution cannot be optimal as it is not even a local minimum.

We conclude that in the region of sufficiently large magnetizations—i.e., $y\geqslant 1/3$—the OW states (with no NN pairs of spins "down") maximize the NN entanglement locally; i.e., we cannot increase the NN entanglement by allowing *small* admixtures of states with NN pairs of spins "down." For smaller magnetizations—i.e., $0\leqslant y<1/3$—the states that maximize the NN entanglement necessarily contain NN pairs of spins "down."

Note that there is a simple physical interpretation of the critical fraction 1/3 of spins "down": it allows all spin ups to be paired, without requiring spin-"down" pairs. This corresponds to "zero magnetization" in the "composite-particle" *XY* model of O'Connor and Wootters, where each spin "down" is forced to have a spin "up" as neighbor, such that this pair can be seen as an entity [31]. Despite this simple interpretation of the value 1/3, we have not been able to provide a simple physical explanation for it. However, it is completely natural to expect that as the fraction of spins "down" is increased (y decreased) the restriction that spins "down" not be allowed to be nearest neighbors becomes relatively more important. Eventually the restriction becomes too severe and the optimum is found in a state that breaks it.

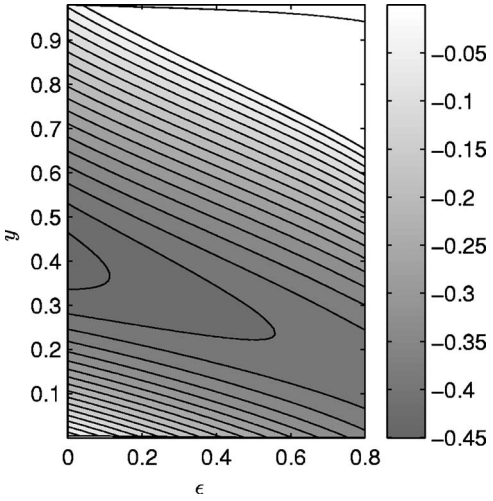

FIG. 4. $H_{Wolf}(\epsilon,y)$ calculated numerically from the recursion formula (40). For each b we find the expansion coefficients of H_{Wolf} and y up to the 14th order in $\epsilon=1/|\Delta|$. The overall optimal state has $y=0.398\,316\ldots$. From Sec. VII B we know that for all $y>1/3$, $\epsilon=0$ is a local minimum for H_{Wolf} and this plot indicates that it is also a global one.

A possible avenue to making these arguments more quantitative goes via Eq. (39) in our previous work [34]. There the possible gain in C by allowing small admixtures of states with spin-"down" pairs is evaluated in terms of the optimal restricted state without such pairs and it should in principle be possible to use this to give an alternative and perhaps more transparent derivation of Eq. (45). We leave this for future investigations.

C. Higher orders

The recursion formula (40) is also well suited for numerical calculations. In Fig. 4 we show a contour plot based on such a calculation including all terms up to 14th order in $\epsilon=1/|\Delta|$. The plot indicates that the calculation in Sec. VII B gives a global answer; i.e., for all $y\geqslant 1/3$, the optimal state has no neighboring spins "down."

Since we perform here the perturbative calculation up to the 14th order, we expect that this calculation allows us also to obtain some information about the region of $y<1/3$. From Fig. 4 (or more precisely from the numerical data), one can read off the optimal value of ϵ—i.e., optimal value of Δ. Solving the Bethe ansatz integral equation for this value of Δ we can recover in this way the full information about the corresponding optimal quantum state.

VIII. CONCLUSIONS

In this paper we have studied the question posed by O'Connor and Wootters concerning translationally invariant states of N qubits with maximal nearest-neighbor concurrence. We have answered this question for $N\to\infty$ using the mapping of the problem onto the search for ground states of a certain family of "parent" Hamiltonians, described by the *XXZ* model. Using the analytic Bethe ansatz solutions of the

XXZ model in the limit $N \to \infty$ (combining analytic results of low-order perturbation theory and a numerical calculation of the 14th-order perturbation theory) we have proved that (i) for a given number of spins "down"—i.e. a given magnetization y larger than $1/3$—the states that maximize the NN concurrence coincide with the ones obtained by O'Connor and Wootters—i.e., do not have NN pairs of spins "down." (ii) For small magnetizations, more explicitly for $0 \leqslant y \leqslant 1/3$, the states that maximize the NN concurrence do contain nearest-neighbor pairs of spins "down." (iii) In particular, the state that maximizes the NN concurrence without constraint on y belongs to the family introduced by O'Connor and Wootters. Our results shed more light on the subtle relations between entanglement in spin-1/2 models and the ferromagnetic and antiferromagnetic character of spin-spin interactions. In the Appendix we present some simple bounds on the optimal magnetic field that corresponds to the maximal NN concurrence.

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APPENDIX: BOUND ON THE OPTIMAL MAGNETIC FIELD

If one keeps y fixed and uses $\mathcal{H}$ to parametrize the s curve instead of s, one gets

$$\frac{dE_{\mathrm{GS}}}{d\mathcal{H}} = -\frac{d\Delta}{d\mathcal{H}}\frac{1}{2}[1+\langle\sigma_z\sigma_z\rangle] - y$$
$$= 2\frac{\mathcal{H}}{\sqrt{\mathcal{H}^2+1}}P + \left(\frac{\mathcal{H}}{\sqrt{\mathcal{H}^2+1}} - 1\right)y,$$

where P is the probability of two neighboring spins being both "down."

Demanding that $\frac{dE_{\mathrm{GS}}}{d\mathcal{H}}=0$, we find

$$\mathcal{H}_{\mathrm{opt}} = \pm\, y/(2\sqrt{P}\sqrt{P+y}),$$

where $\mathcal{H}_{\mathrm{opt}}$ is the optimal magnetic field. Obviously, $\mathcal{H}_{\mathrm{opt}}=0$ iff $y=0$.

Using a simple bound on P,

$$P \leqslant (y+1)/2 \text{ in the limit } N \to \infty,$$

we obtain a lower bound on $\mathcal{H}_{\mathrm{opt}}$:

$$\mathcal{H}_{\mathrm{opt}} \geqslant y/(\sqrt{y+1}\sqrt{3y+1}).$$

This bound does not work well for $y>1/3$, because it gives a finite bound, maximized for $y=1$ when we find $\mathcal{H}_{\mathrm{opt}} \geqslant 1/(2\sqrt{2})$, whereas we know that in this regime of y's $\mathcal{H}_{\mathrm{opt}}=\infty$. For smaller values of $y<1/3$, both the optimal ϵ (i.e., Δ; see Fig. 4), as well as the optimal $\mathcal{H}_{\mathrm{opt}}$, attain finite values, so that the bound might become more useful. In particular, the results of Fig. 4 suggest that as y approaches zero, the optimal ϵ approaches 1 more or less linearly, as $1-(1/3)^{-1}y$, which in turn implies that the optimal Δ approaches -1 as $-1-3y$. Thus for small y and small $\Delta+1$, the bound becomes $\mathcal{H}_{\mathrm{opt}} \geqslant -\frac{1}{3}(1+\Delta)$, which already is not obvious (compare Fig. 1).

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