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# Entanglement of formation for one-dimensional magnetic systems with defects

Zhen Huang, Omar Osenda, Sabre Kais\*

Department of Chemistry, Purdue University, West Lafayette, IN 47907, USA Received 3 November 2003; received in revised form 10 January 2004; accepted 12 January 2004 Communicated by R. Wu

#### Abstract

We present a study of the entanglement of formation for one-dimensional magnetic systems with defects. The concurrence was used as a measure of entanglement. Rather than locating the impurity at one site in the chain, there is a Gaussian distribution of disorder near a particular location. We demonstrate that the entanglement can be tuned by varying the strength of the external magnetic field and the distribution of impurities. The concurrence is a maximum close to the critical point, where a quantum phase transition occurs, and for certain parameters can be tuned to zero above the critical point. © 2004 Elsevier B.V. All rights reserved.

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## 1. Introduction

Quantum entanglement is regarded as the resource of quantum information processing with no classical analog [1–4]. The corresponding investigation is currently a very active area of research [5–10] due to its potential applications in quantum communication, such as quantum teleportation [11,12], superdense coding [13], quantum key distribution [14], telecoloning [15] and decoherence in quantum computers [16,17].

The study of the entanglement as a function of the parameters in a system might be of great importance in quantum computation and communication. Osterloh et al. [18] connected the theory of critical phenomena with quantum information by exploring the entangling resources of a system close to its quantum critical point. They demonstrated, for a class of one-dimensional magnetic systems modeled by the XY model, that entanglement shows scaling behavior in the vicinity of the transition point. Recently [19], we have demonstrated that for such a class of one-dimensional magnetic systems entanglement can be controlled and tuned by varying the anisotropy parameter in the XY Hamiltonian and by introducing impurities into the systems. In particular, for certain parameters, the entanglement is zero up to a critical point  $\lambda_c$ , where a quantum phase transition occurs, and is different from zero above  $\lambda_c$ . Although, great interest attaches to three-dimensional lattices, the properties of one-dimensional

Corresponding author.

E-mail address: kais@purdue.edu (S. Kais).

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magnetic systems with anisotropic coupling and impurities are of both experimental and theoretical significance [20–23].

In this Letter, we consider a set of localized spin-1/2 particles coupled through exchange interaction and subject to an external magnetic field in the presence of impurities in the form of Gaussian distributions along the chain.

# 2. Solution of the XY model

In this section, we consider the numerical solution of the XY model on a one-dimensional lattice with N sites in a transverse magnetic field and impurities. The Hamiltonian for such a system is given by

$$H = -\frac{1+\gamma}{2} \sum_{i=1}^{N} J_{i,i+1} \sigma_i^x \sigma_{i+1}^x - \frac{1-\gamma}{2} \sum_{i=1}^{N} J_{i,i+1} \sigma_i^y \sigma_{i+1}^y - \sum_{i=1}^{N} h_i \sigma_i^z, \tag{1}$$

where  $J_{i,i+1}$  is the exchange interaction between sites *i* and *i* + 1,  $h_i$  is the strength of the external magnetic field on site *i*,  $\sigma^a$  are the Pauli matrices (a = x, y, z),  $\gamma$  is the degree of anisotropy and *N* is the number of sites. We assume cyclic boundary conditions, so that

$$\sigma_{N+1}^{x} = \sigma_{1}^{x}, \qquad \sigma_{N+1}^{y} = \sigma_{1}^{y}, \qquad \sigma_{N+1}^{z} = \sigma_{1}^{z}.$$
 (2)

The standard procedure used to solve Eq. (1) is to transform the spin operators into fermionic operators [24]. Let us define the raising and lowering operators  $a_i^+$ ,  $a_i^-$ ,

$$a_i^+ = \frac{1}{2} (\sigma_i^x + i\sigma_i^y), \qquad a_i^- = \frac{1}{2} (\sigma_i^x - i\sigma_i^y)$$
 (3)

in terms of which the Pauli matrices are

$$\sigma_i^x = a_i^+ + a_i^-, \qquad \sigma_i^y = \frac{a_i^+ - a_i^-}{i}, \qquad \sigma_i^z = 2a_i^+ a_i^- - I.$$
(4)

Then, we introduce Fermi operators  $c_i, c_i^+$ , defined by

$$a_i^- = \exp\left(-i\pi \sum_{j=1}^{i-1} c_j^+ c_j\right) c_i, \qquad a_i^+ = c_i^+ \exp\left(i\pi \sum_{j=1}^{i-1} c_j^+ c_j\right).$$
(5)

So that, the Hamiltonian assumes the following quadratic form

$$H = -\sum_{i=1}^{N} J_{i,i+1} \Big[ (c_i^+ c_{i+1} + \gamma c_i^+ c_{i+1}^+) + \text{h.c.} \Big] - 2\sum_{i=1}^{N} h_i \Big( c_i^+ c_i - \frac{1}{2} \Big).$$
(6)

In this study the exchange interaction has the form  $J_{i,i+1} = J(1 + \alpha_{i,i+1})$ , where  $\alpha$  introduces the impurity in a Gaussian form centered at  $\frac{N+1}{2}$  with strength or height  $\zeta$ ,

$$\alpha_{i,i+1} = \zeta \exp\left\{-\epsilon \left(i - \frac{N+1}{2}\right)^2\right\}.$$
(7)

The external magnetic field takes the form  $h_i = h(1 + \beta_i)$ , where  $\beta$  has the following Gaussian form

$$\beta_i = \xi \exp\left\{-\epsilon \left(i - \frac{N+1}{2}\right)^2\right\}.$$
(8)

When  $\alpha = \beta = 0$  we recover the pure case. For both distributions of the impurity and the magnetic field, we fixed the value of the width of the distribution at  $\epsilon = 0.1$  in all the calculations.

By introducing the dimensionless parameter  $\lambda = J/2h$ , the symmetrical matrix A

and the antisymmetrical **B** 

the Hamiltonian becomes

$$H = \sum_{i,j=1}^{N} \left[ c_i^+ A_{i,j} c_j + \frac{1}{2} \left( c_i^+ B_{i,j} c_j^+ + \text{h.c.} \right) \right].$$
(11)

The quadratic Hamiltonian can be diagonalized by making a linear transformation of the fermionic operators,

$$\eta_k = \sum_{i=1}^N g_{ki}c_i + h_{ki}c_i^+, \qquad \eta_k^+ = \sum_{i=1}^N g_{ki}c_i^+ + h_{ki}c_i, \qquad (12)$$

where  $g_{ki}$  and  $h_{ki}$  are real. Then the Hamiltonian becomes

$$H = \sum_{k}^{N} \Lambda_k \eta_k^+ \eta_k + \text{const},$$
(13)

with the following two coupled matrix equations which satisfy

$$\phi_{\mathbf{k}}(\mathbf{A} - \mathbf{B}) = \mathbf{\Lambda}_{\mathbf{k}}\psi_{\mathbf{k}}, \qquad \psi_{k}(\mathbf{A} + \mathbf{B}) = \mathbf{\Lambda}_{\mathbf{k}}\phi_{\mathbf{k}}, \tag{14}$$

where the components of the two column vectors  $\phi_{ki}$  and  $\psi_{ki}$  are given by

$$\phi_{ki} = g_{ki} + h_{ki}, \qquad \psi_{ki} = g_{ki} - h_{ki}. \tag{15}$$

Finally, the ground state of the system  $|\Psi_0\rangle$  can be written as

$$\eta_k |\Psi_0\rangle = 0. \tag{16}$$

# 3. Spin-spin correlation functions

A great deal of information about the preponderance of up-spin on one sublattice to down-spin on the other sublattice, can be obtained by investigating the different spin–spin correlation functions and the average magnetization per spin [24].

The spin-spin correlation functions for ground state are defined as

$$S_{lm}^{x} = \frac{1}{4} \langle \Psi_0 | \sigma_l^x \sigma_m^x | \Psi_0 \rangle, \tag{17}$$

$$S_{lm}^{\nu} = \frac{1}{4} \langle \Psi_0 | \sigma_l^{\nu} \sigma_m^{\nu} | \Psi_0 \rangle, \tag{18}$$

$$S_{lm}^{z} = \frac{1}{4} \langle \Psi_0 | \sigma_l^z \sigma_m^z | \Psi_0 \rangle, \tag{19}$$

and the average magnetization per spin

$$M_i^z = \frac{1}{2} \langle \Psi_0 | \sigma_i^z | \Psi_0 \rangle.$$
<sup>(20)</sup>

In order to calculate these correlation functions, we must first calculate the following quantities:

$$\langle \Psi_0 | A_i A_j | \Psi_0 \rangle, \qquad \langle \Psi_0 | B_i B_j | \Psi_0 \rangle, \qquad \langle \Psi_0 | B_i A_j | \Psi_0 \rangle \tag{21}$$

where  $A_i = c_i^+ + c_i$  and  $B_i = c_i^+ - c_i$ . From Eqs. (12) and (15), since  $\psi_k$  and  $\phi_k$  are orthonormal, we can get

$$A_{i} = \sum_{k}^{N} (\eta_{k} + \eta_{k}^{+}) \phi_{ki}, \qquad B_{i} = \sum_{k}^{N} (\eta_{k}^{+} - \eta_{k}) \psi_{ki}.$$
(22)

Thus, using Eq. (16), we obtain

$$\langle \Psi_0 | A_i A_j | \Psi_0 \rangle = \sum_k^N \phi_{ki} \phi_{kj} = \delta_{ij}, \qquad (23)$$

$$\langle \Psi_0 | B_i B_j | \Psi_0 \rangle = -\sum_k^N \psi_{ki} \psi_{kj} = -\delta_{ij}, \qquad (24)$$

$$\langle \Psi_0 | B_i A_j | \Psi_0 \rangle = -\langle \Psi_0 | A_j B_i | \Psi_0 \rangle = -\sum_k^N \psi_{ki} \phi_{kj} \equiv G_{ij}.$$
(25)

Using Wick's theorem [25] we obtain

$$S_{lm}^{x} = \frac{1}{4} \begin{pmatrix} G_{l,l+1} & G_{l,l+2} & \cdots & G_{l,m} \\ \vdots & \vdots & \ddots & \vdots \\ G_{m-1,l+1} & G_{m-1,l+2} & \cdots & G_{m-1,m} \end{pmatrix},$$
(26)

$$s^{y} = \begin{pmatrix} G_{l+1,l} & G_{l+1,l+1} & \dots & G_{l+1,m-1} \\ \vdots & \vdots & \vdots & \vdots \\ \vdots & \vdots & \vdots & \vdots \end{pmatrix}$$
(27)

$$S_{lm}^{*} = \frac{1}{4} \begin{pmatrix} \vdots & \vdots & \ddots & \vdots \\ G_{m,l} & G_{m,l+1} & \dots & G_{m,m-1} \end{pmatrix},$$
(27)

$$S_{lm}^{z} = \frac{1}{2}(G_{ll}G_{mm} - G_{ml}G_{lm}),$$
(28)

$$M_i^z = \frac{1}{2}G_{ii}.$$

## 4. Entanglement of formation

The concept of entanglement of formation is related to the amount of entanglement needed to prepare the state  $\rho$ , where  $\rho$  is the density matrix. It was shown by Wootters [7] that

$$E(\rho) = \mathcal{E}(C(\rho)), \tag{30}$$

where the function  $\mathcal{E}$  is given by

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$$\mathcal{E} = h\left(\frac{1+\sqrt{1-C^2}}{2}\right),\tag{31}$$

where  $h(x) = -x \log_2 x - (1 - x) \log_2(1 - x)$ , and *C* is the concurrence. Since  $\mathcal{E}(C)$  is monotonically increasing and ranges from 0 to 1 as *C* goes from 0 to 1, so the one can take the concurrence as a measure of entanglement in its own right [6]. The concurrence *C* is given by [7]

$$C(\rho) = \max\{0, \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4\}.$$
(32)

For a general state of two qubits,  $\lambda_i$ 's are the eigenvalues, in decreasing order, of the Hermitian matrix

$$R \equiv \sqrt{\sqrt{\rho}\,\tilde{\rho}\sqrt{\rho}},\tag{33}$$

where  $\rho$  is the density matrix and  $\tilde{\rho}$  is the spin-flipped state defined as

$$\tilde{\rho} = (\sigma_y \otimes \sigma_y) \rho^* (\sigma_y \otimes \sigma_y), \tag{34}$$

where the  $\rho^*$  is the complex conjugate of  $\rho$  and is taken in the standard basis, which for a pair of spin- $\frac{1}{2}$  particles is  $\{|\uparrow\uparrow\rangle, |\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle, |\downarrow\downarrow\rangle$ . Alternatively, the  $\lambda_i$ 's are the square roots of the eigenvalues of the non-Hermitian  $\rho\bar{\rho}$ .

The structure of the reduced density matrix follows from the symmetry properties of the Hamiltonian. However, for this case the concurrence C(i, j) depends on i, j and the location of the impurity and not only on the difference |i - j| as for the pure case. Using the operator expansion for the density matrix and the symmetries of the Hamiltonian [26] lead to the general form

$$\rho = \begin{pmatrix} \rho_{1,1} & 0 & 0 & \rho_{1,4} \\ 0 & \rho_{2,2} & \rho_{2,3} & 0 \\ 0 & \rho_{2,3} & \rho_{3,3} & 0 \\ \rho_{1,4} & 0 & 0 & \rho_{4,4} \end{pmatrix},$$
(35)

with

$$\lambda_{a} = \sqrt{\rho_{1,1}\rho_{4,4}} + |\rho_{1,4}|, \qquad \lambda_{b} = \sqrt{\rho_{2,2}\rho_{3,3}} + |\rho_{2,3}|, \lambda_{c} = \left|\sqrt{\rho_{1,1}\rho_{4,4}} - |\rho_{1,4}|\right|, \qquad \lambda_{d} = \left|\sqrt{\rho_{2,2}\rho_{3,3}} - |\rho_{2,3}|\right|.$$
(36)

Using the definition  $\langle A \rangle = \text{Tr}(\rho A)$ , we can express all the matrix elements in the density matrix in terms of different spin–spin correlation functions:

$$\rho_{1,1} = \frac{1}{2}M_l^z + \frac{1}{2}M_m^z + S_{lm}^z + \frac{1}{4},\tag{37}$$

$$\rho_{2,2} = \frac{1}{2}M_l^z - \frac{1}{2}M_m^z - S_{lm}^z + \frac{1}{4},\tag{38}$$

$$\rho_{3,3} = \frac{1}{2}M_m^z - \frac{1}{2}M_l^z - S_{lm}^z + \frac{1}{4},\tag{39}$$

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$$\rho_{4,4} = -\frac{1}{2}M_l^z - \frac{1}{2}M_m^z + S_{lm}^z + \frac{1}{4},\tag{40}$$

$$\rho_{2,3} = S_{lm}^x + S_{lm}^y, \tag{41}$$

$$\rho_{1,4} = S_{lm}^x - S_{lm}^y. \tag{42}$$

## 5. Results and discussions

For the sake of clarity, we focus our discussions on the transverse Ising model, which arises as the limit  $\gamma \rightarrow 1$ . This system is the simplest quantum lattice system to exhibit a quantum phase transition. For the pure case with  $\alpha = 0$ , Osborne and Nielsen [26] argue that the Ising model provide the clearest evidence for the conjecture that the critical point corresponds to the situation where the lattice is most entangled [26]. Our goal is to examine this system in the presence of impurities. In Fig. 1 we show the results of the nearest neighbor concurrence and its derivative, between the sites 49 and 50, as a function of the parameter  $\lambda = J/2h$  for different Gaussian distributions of the impurity (see Eq. (7)) and for different strengths of the external magnetic field (see Eq. (8)). In the left panel of Fig. 1, the parameter  $\zeta$  of the Gaussian distribution of the impurity was varied from the pure case with  $\zeta = 0$  to  $\zeta = 1$ . In the right panel of Fig. 1, the parameter  $\xi$  of the Gaussian distribution for the external magnetic field was varied from  $\xi = 0$  to  $\xi = 1$ .

One can see that the concurrence is close to zero above the critical point  $\lambda_c$  and a maximum close to  $\lambda_c$ . As  $\zeta$  increases the concurrence tends to increase faster and the  $\lambda_m$ , where concurrence approaches maximum, shift to zero very rapidly. However, the concurrence increases slowly and the  $\lambda_m$  tends to move to infinity by increasing the value of the parameter  $\xi$ . The derivative of concurrence for different values of  $\zeta$  and  $\xi$  with respect to  $\lambda$ , is also presented in the Fig. 1. We find that the derivative of concurrence starts at a maximum value, then approaches a



Fig. 1. The nearest neighbor concurrence C(49, 50) and its derivative for different values of the Gaussian distribution in the external magnetic field,  $\xi$ , and the impurities,  $\zeta$ , as a function of the reduced coupling constant  $\lambda$ , the system size N = 101 and the anisotropy parameter  $\gamma = 1$ .



Fig. 2. The spin–spin correlation functions and the average magnetization per spin for different Gaussian distributions in the impurities, with the parameter  $\zeta = 0.0, 0.1, 0.5, 1$ .

minimum at the critical point and finally disappears in the limit  $\lambda \to \infty$ . For the pure case, the critical point  $\lambda_c = 1$ . But it shifts to zero for increasing values of  $\zeta$  and to infinity for increasing values of  $\xi$ .

In order to examine the change of the critical point as the parameters  $\zeta$  and  $\xi$  varies, we calculated the three spin–spin correlation functions  $S_{lm}^x$ ,  $S_{lm}^y$ ,  $S_{lm}^z$  and the average magnetization per spin  $M_i^z$ . Fig. 2 shows the behavior of different spin–spin correlation functions for different values of the parameter  $\zeta$ . For the pure Ising model at  $N = \infty$ , the system exhibit a quantum phase transition at  $\lambda_c = 1$ . The spin–spin correlation function  $S^x$  is different from zero for  $\lambda > 1$  and it vanishes at the transition. On the contrary the magnetization along the z direction is different from zero for any value of  $\lambda$ . As expected, the spin–spin correlation functions  $\langle S^y \rangle$  and  $\langle S^z \rangle$  are almost zero for all values of  $\lambda$ . As the value of the parameter  $\zeta$  increases, the magnetization  $M^z$  becomes different from zero for smaller values of  $\lambda_c < 1$ . Similar analysis shows that on the contrary the spin–spin correlation function  $\langle S^x \rangle$  becomes different from zero for larger values of  $\lambda_c > 1$  as the value of the parameter  $\xi$  increases.

Up to now we examined the nearest neighbor concurrence C(49, 50) with different Gaussian distributions for impurities and strengths of the magnetic field. It is interesting to see the effect of the different Gaussian distributions on the concurrence for the rest of the sites in the chain. Fig. 3 shows the nearest neighbor concurrence for all sites in the chain with different  $\zeta$  at  $\lambda = 0.2$  and  $\lambda = 0.9$ . At  $\lambda = 0.2$ , the nearest neighbor concurrences near the center of the Gaussian distribution increases and reaches their maximum when  $\zeta \approx 2$ . Then they become smaller as  $\zeta$  further increases. When  $\zeta \approx 20$ , the concurrence near the center of Gaussian distribution approaches zero. When  $\zeta > 2$ the concurrence peak splits into two. The height of the two peaks decrease by increasing  $\zeta$ , until they disappear for  $\zeta \gg 1$ . However, at  $\lambda = 0.9$  the nearest neighbor concurrences near the center of Gaussian distribution always decrease when  $\zeta$  increase. This fact indicates that the nearest-neighbor concurrence in the one-dimensional Ising model can be controlled by tuning the impurity for specific external magnetic field.

To examine the effect of the Gaussian distribution in the magnetic field on all sites of the chain, we show in Fig. 4 the results for the nearest neighbor concurrence C(i, i + 1) for all the sites for  $\lambda = 0.5$  and  $\lambda = 1.5$ . For  $\lambda = 0.5$ , the concurrences near the center of the Gaussian distribution can be tuned down by increasing the value of  $\xi$ . However, the concurrence for the other sites approach zero when  $\xi \gg 1$ . For  $\lambda = 1.5$  the results similar to one



Fig. 3. The nearest neighbor concurrence C(i, i + 1) for all sites on the chain with system size N = 101 for  $\lambda = 0.2$  and  $\lambda = 0.9$ . The curves correspond to different values of  $\zeta = 0.1, 2.0, 4.0, 20.0$ .



Fig. 4. The nearest neighbor concurrence C(i, i + 1) for all sites on the chain with system size N = 101 for  $\lambda = 0.5$  and  $\lambda = 1.5$ . The curves correspond to different values of  $\xi = 0.1, 1.0, 5.0, 20.0$ .

in Fig. 3 for the case with impurity at  $\lambda = 0.2$ . The concurrence peak at the center of the distribution splits into two by increasing the value of  $\xi$ .

In summary, we have focused our calculations on the Ising model,  $\gamma \rightarrow 1$ , although the method for the numerical solution is general and cover the XY model. In our previous publication [19] we examined the change of entanglement as the degree of the anisotropy  $\gamma$  varies between zero and one. The concurrence was used as a measure of entanglement. In this Letter, rather than locating the impurity at one site in the chain [19], we introduce a Gaussian distribution of disorder near a particular location. We have shown that the entanglement can be tunned by varying the strengths of the magnetic field and the impurity distribution in the system. The concurrence is maximum close to  $\lambda_c$  and can be tuned to zero above the critical point.

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