Localizable entanglement in antiferromagnetic spin chains

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Antiferromagnetic spin chains play an important role in condensed matter and statistical mechanics. Recently *XXX* spin chain was discussed in relation to information theory. Here we consider localizable entanglement. It is how much entanglement can be localized on two spins by performing local measurements on other individual spins (in a system of many interacting spins). We consider the ground state of antiferromagnetic spin chain. We study localizable entanglement [represented by concurrence] between two spins. It is a function of the distance. We start with isotropic spin chain. Then we study effects of anisotropy and magnetic field. We conclude that anisotropy increases the localizable entanglement. We discovered high sensitivity to a magnetic field in cases of high symmetry. We also evaluated concurrence of these two spins before the measurement to illustrate that the measurement raises the concurrence.

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I. INTRODUCTION

Spin chains play an important role in solid state physics [1–6]. For example, inelastic neutron scattering on $SrCuO_2$ [7] can be explained by spin 1/2 Heisenberg chain [8]. Spin chains are also important for information theory. Recently, many-body systems have attracted a lot of attention in the field of quantum information [9–12]. Special attention has been paid to the entanglement in these systems. Entanglement plays the main role as a physical resource for quantum information and quantum computation. There is a lot in common between quantum statistical mechanics and quantum information theory. The role of phase transitions for quantum information was emphasized in Ref. [11]. The most direct relation between correlation functions and entanglement was discovered by Verstraete, Popp, and Cirac (VPC) in Ref. [9]. They found that correlation function provides a bound for localizable entanglement (LE).

The LE of two spins is defined as the maximal amount of entanglement that can be localized on two marked spins on average by doing local measurements on the rest of the spins (assisting spins). Here we assume that we consider a pure state $|\phi\rangle$ of all these spins. The LE has an operational meaning applicable to situations in which one would like to concentrate as much entanglement as possible between two particular particles out of multi-particle entangled state. Good examples are quantum repeater [13] and spinotronics (microelectronic devices that function by using the spin of the electron) [14]. Let us consider an example of N qubits in GHZ state:

$$|GHZ\rangle = \frac{1}{\sqrt{2}}(|00\ldots0\rangle + |11\ldots1\rangle). \tag{1}$$

We can measure assisting qubits in $|\pm\rangle$ basis. This will force two marked spins into a Bell state (maximally entangled state of two qubits).

Let us proceed to the formal definition for localizable entanglement E_{ij} between two spins marked by i and j. Consider a pure state of N spins $|\phi\rangle$ [it is normalized $\langle\phi|\phi\rangle=1$]. Every measurement basis specifies an ensemble of pure states $\mathcal{E}=\{p_s,|\psi_s\rangle\}$. The index s enumerates different measurement outcomes. It runs through $2^{(N-2)}$ values. Here $|\psi_s\rangle$ is a two-spin state after the measurement and p_s is its probability. The LE is defined as

$$E_{ij} = \max_{\mathcal{E}} \sum_s p_s E(|\psi_s\rangle). \tag{2}$$

Here $E(|\psi_s\rangle)$ is the entanglement of $|\psi_s\rangle$, characterized by concurrence. The concurrence C was suggested by Wooters [15] as a measure of entanglement [16]. By definition it is $0\leqslant C\leqslant 1$. VPC noticed that it is in particular a convenient measure for LE. It is important for us that concurrence for two qubits state $|\phi\rangle=a|00\rangle+b|01\rangle+c|10\rangle+d|11\rangle$ coincides with maximum correlation $C(|\phi\rangle)=2|ad-bc|$.

It is difficult to calculate LE. Instead, VPC found bounds for LE. The upper bound comes out of considering a global (joint) measurement on all assisting spins. It can be related to the entanglement of assistance, which is the maximum entanglement over all possible states of N spins consistent with the density matrix of two marked spins. It was introduced by DiVincenzo, Fuchs, Mabuchi, Smolin, Thapliyal, and Uhlmann [17]. A simple formula for entanglement of assistance was found in Ref. [18]. Let us denote the density matrix of two marked spins by ρ_{ij}. Matrix X is a square root of the density matrix: $\rho_{ij}=XX^\dagger$. The entanglement of assistance measured by concurrence is given by the trace norm $\mathrm{tr}[X^T(\sigma_y\otimes\sigma_y)X]$. Hence, the upper bound of LE is

$$E_{ij} \leqslant \frac{\sqrt{s_+^{ij}} + \sqrt{s_-^{ij}}}{2}, \tag{3}$$

where

$$s_\pm^{ij} = (1 \pm \langle\phi|\sigma_z^{(i)}\sigma_z^{(j)}|\phi\rangle)^2 - (\langle\phi|\sigma_z^{(i)}|\phi\rangle \pm \langle\phi|\sigma_z^{(j)}|\phi\rangle)^2.$$

The lower bound on LE is expressed in terms of correlation functions:

$$Q^{ij}_{\alpha\beta} = \langle\langle \phi|\sigma^{(i)}_{\alpha}\sigma^{(j)}_{\beta}|\phi\rangle\rangle \equiv \langle \phi|\sigma^{(i)}_{\alpha}\sigma^{(j)}_{\beta}|\phi\rangle - \langle \phi|\sigma^{(i)}_{\alpha}|\phi\rangle\langle \phi|\sigma^{(j)}_{\beta}|\phi\rangle. \tag{4}$$

The lower bound on LE is based on the following observation [9]. Given a state of N spins with fixed correlation functions $Q^{ij}_{\alpha\beta}$ between two spins (marked by i and j) and directions α and β, there exist directions in which one can measure other spins (assisting spins), such that this correlation does not decrease. Using this observation, VPC found a lower bound for LE:

$$E_{ij} \geqslant \max_{\alpha}(|Q^{ij}_{\alpha\alpha}|). \tag{5}$$

VPC explicitly evaluated these bounds for the ground state of the Ising model and showed that actual value of LE is close to the lower bound.

In this paper we consider the ground state of infinite antiferromagnetic XXX spin chain at zero temperature. We also consider anisotropic version: XXZ chain. We calculated the concurrence before the measurement (see Appendix A) and compare it to LE. Measurement raises the concurrence.

II. *XXX* ANTIFERROMAGNETIC SPIN CHAIN

The Hamiltonian for antiferromagnetic XXX spin chain can be written as

$$H^0_{XXX} = \sum_m \{\sigma^{(m)}_x\sigma^{(m+1)}_x + \sigma^{(m)}_y\sigma^{(m+1)}_y + \sigma^{(m)}_z\sigma^{(m+1)}_z\}. \tag{6}$$

Here $\sigma^{(m)}_x,\sigma^{(m)}_y,\sigma^{(m)}_z$ are Pauli matrix, which describe spin operators on mth lattice site. Summation goes through the whole infinite lattice. The density of the Hamiltonian is a linear function of the swap gate.

Hans Bethe found eigenfunctions of the Hamiltonian of the model in 1931 [19]. The ground state $|\phi\rangle$ was found by Hulten in Ref. [20]. We shall normalize it to 1. Correlations are defined as averages with respect to the ground state. They are isotropic

$$\langle \phi|\sigma^{(i)}_{\alpha}\sigma^{(j)}_{\beta}|\phi\rangle = \delta^{\alpha\beta}\langle \phi|\sigma^{(i)}_{z}\sigma^{(j)}_{z}|\phi\rangle. \tag{7}$$

There is no magnetization σ_α ($\alpha = x,y$ or z),

$$\sigma_\alpha = \langle \phi|\sigma^{(j)}_{\alpha}|\phi\rangle = 0. \tag{8}$$

This simplifies the lower bound (5) of LE [21]:

$$1 \geqslant E_{ij} \geqslant \langle \phi|\sigma^{(i)}_{z}\sigma^{(j)}_{z}|\phi\rangle. \tag{9}$$

Let us now use the explicit expression for correlations $\langle \phi|\sigma^{(i)}_{z}\sigma^{(j)}_{z}|\phi\rangle$ to calculate the lower bound:

$$\langle \phi|\sigma^{(m)}_{z}\sigma^{(m+1)}_{z}|\phi\rangle = \frac{1}{3} - \frac{4}{3}\ln 2 \simeq -0.5908629072, \tag{10}$$

$$\langle \phi|\sigma^{(m)}_{z}\sigma^{(m+2)}_{z}|\phi\rangle = \frac{1}{3} - \frac{16}{3}\ln 2 + 3\zeta(3) \simeq 0.2427190798, \tag{11}$$

$$\begin{aligned}\langle \phi|\sigma^{(m)}_{z}\sigma^{(m+3)}_{z}|\phi\rangle &= \frac{1}{3} - 12\ln 2 + \frac{74}{3}\zeta(3) - \frac{56}{3}\zeta(3)\ln 2 \\ &\quad - 6\zeta(3)^2 - \frac{125}{6}\zeta(5) + \frac{100}{3}\zeta(5)\ln 2 \\ &\simeq -0.2009945090,\end{aligned} \tag{12}$$

$$\begin{aligned}\langle \phi|\sigma^{(m)}_{z}\sigma^{(m+4)}_{z}|\phi\rangle &= \frac{1}{12} - \frac{16}{3}\ln 2 - 54\ln 2\zeta(3) - \frac{293}{4}\zeta^2(3) \\ &\quad - \frac{875}{12}\zeta(5) + \frac{145}{6}\zeta(3) + \frac{1450}{3}\ln 2\ \zeta(5) \\ &\quad - \frac{275}{16}\zeta(3)\zeta(5) - \frac{1875}{16}\zeta^2(5) + \frac{3185}{64}\zeta(7) \\ &\quad - \frac{1715}{4}\ln 2\zeta(7) + \frac{6615}{32}\zeta(3)\zeta(7) \\ &\simeq 0.0346527769.\end{aligned} \tag{13}$$

It took a long time to evaluate correlations functions. Nearest neighbor correlation can be extracted from the ground state energy [20]. Next to nearest neighbor correlation was calculated by Takahashi in 1977, see Ref. [22]. Recently it was established that all correlations can be expressed as polynomials of ln 2 and the values of Riemann zeta function [23] at odd arguments [24–29]. These polynomials have only rational coefficients. Third neighbor correlation was calculated by Sakai, Shiroishi, Nishiyama, and Takahashi, see [30]. These results give us the following bounds for localizable entanglement [LE]:

$$E_{j,j+1} \geqslant 0.5908629072, \tag{14}$$

$$E_{j,j+2} \geqslant 0.2427190798, \tag{15}$$

$$E_{j,j+3} \geqslant 0.2009945090. \tag{16}$$

$$E_{j,j+4} \geqslant 0.0346527769. \tag{17}$$

At large distances correlation functions exhibit critical behavior. Asymptotic was obtained in [31] and [32]

$$\langle \phi|\sigma^{(i)}_{z}\sigma^{(j)}_{z}|\phi\rangle \to (-1)^{i-j}\left\{\frac{(2\ln|i-j|)^{1/2}}{(\pi)^{3/2}|i-j|}\right\}. \tag{18}$$

This helps us to estimate localizable entanglement asymptotically for two spins, which are far away, i.e., $|i-j| \to \infty$:

$$E_{ij} \geqslant \left\{\frac{(2\ln|i-j|)^{1/2}}{(\pi)^{3/2}|i-j|}\right\}. \tag{19}$$

Even better, but more complicated expression for lower bound of LE, can be extracted from the paper [33]:

$$E_{ij} \geq \sqrt{\frac{2}{\pi^3}}\frac{1}{|i-j|\sqrt{g}}\left\{1+\left(\frac{3}{8}-\frac{c}{2}\right)g+\left(\frac{5}{128}-\frac{c}{16}-\frac{c^2}{8}\right)g^2 + \left(\frac{21}{1024}+\frac{7c}{256}-\frac{7c^2}{64}-\frac{c^3}{16}+\frac{13\ \zeta(3)}{32}\right)g^3+O(g^4)\right\} - \frac{(-1)^{|i-j|}}{\pi^2|i-j|^2}\left\{1+\frac{g}{2}+\left(c+\frac{3}{4}\right)\frac{g^2}{2}+\frac{c(c+2)}{2}g^3+O(g^4)\right\} + \ldots . \quad (20)$$

Here the coupling constant g depends on the distance $|i-j|$. It is defined by

$$\sqrt{g}e^{1/g} = 2\sqrt{2\pi}e^{\gamma_E+c}|i-j|. \quad (21)$$

Here $\gamma_E = 0.5772$ is the Euler's constant and c is a parameter [normalization point]. A good choice for c is $c=-1$. This boundary for LE is suitable for the full range of distances. In Appendix A we calculated concurrence before the measurement. It is nonzero only for nearest neighbors, see Ref. [34] and Eq. (A26). Clearly, the measurement raises the concurrence.

III. CRITICAL *XXZ* ANTIFERROMAGNET

Let us consider effects of anisotropy of interaction of spins. The Hamiltonian of the *XXZ* spin chain is

$$\mathbf{H}^0_{XXZ} = -\sum_m \{\sigma_x^{(m)}\sigma_x^{(m+1)} + \sigma_y^{(m)}\sigma_y^{(m+1)} + \ \Delta\,(\sigma_z^{(m)}\sigma_z^{(m+1)} - 1)\}. \quad (22)$$

We shall consider critical regime $(-1 \leq \Delta < 1)$ and we use parametrization:

$$\Delta = \cos(\pi\eta), \quad 0 < \eta < 1. \quad (23)$$

Let us recall that the case $\eta=0$ corresponds to ferromagnetic *XXX*, which we are not considering here. Another case $\eta=1$ corresponds to antiferromagnetic *XXX*, see the previous section.

The case $\eta=2/3$ corresponds to $\Delta=-1/2$. In this case the model admits much simpler solution than generic Bethe Anzats, see Refs. [35–37]. In this case the model is supersymmetric, see Ref. [38].

Later we shall see that all these special cases $\eta=0,2/3,1$ have high sensitivity to magnetic field interacting with spins.

For general values of η (23) there is no magnetization:

$$\sigma_\alpha = \langle\phi|\sigma_\alpha^{(m)}|\phi\rangle = 0. \quad (24)$$

LE is bounded by maximal correlation function:

$$1 \geq E_{ij} \geq \max_\alpha |\langle\phi||\sigma_\alpha^{(i)}\sigma_\alpha^{(j)}|\phi\rangle|. \quad (25)$$

Correlation functions decays as power laws at large distances $\ln|i-j| \gg 1/(2-2\eta)$. Leading terms of correlations are

$$\langle\phi|\sigma_x^{(i)}\sigma_x^{(j)}|\phi\rangle = \langle\phi|\sigma_y^{(i)}\sigma_y^{(j)}|\phi\rangle = F|i-j|^{-\eta},$$

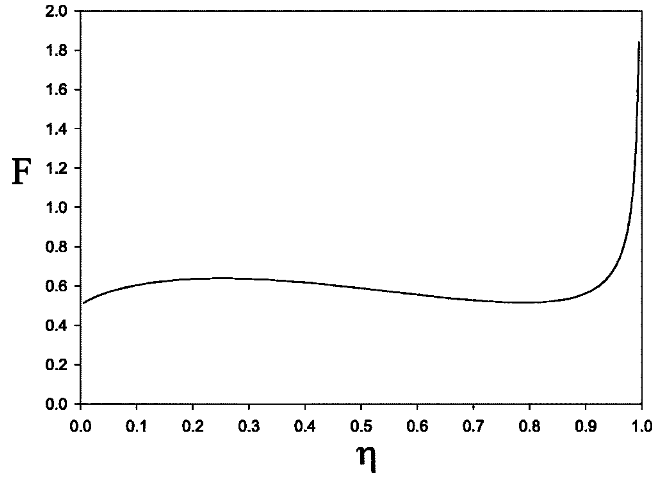

FIG. 1. F (Eq. (28)) vs η.

$$\langle\phi|\sigma_z^{(i)}\sigma_z^{(j)}|\phi\rangle = -\frac{1}{\pi^2\eta}|i-j|^{-2} + A(-1)^{i-j}|i-j|^{-1/\eta}.$$

Many people worked on the subject. Important results are obtained in [31]. A good collection of references can be found in [39], see pages 512, 549–553. Since $0<\eta<1$, it becomes clear that σ_x correlations asymptotically dominate the lower bound:

$$|Q^{ij}_{xx}| = |Q^{ij}_{yy}| > |Q^{ij}_{zz}|. \quad (26)$$

Finally we got the following bound for LE:

$$E_{ij} \geq F|i-j|^{-\eta}. \quad (27)$$

This shows that anisotropy raises the lower bound for LE. The coefficient F was calculated [31,32]

$$F = \frac{1}{2(1-\eta)^2}\left[\frac{\Gamma\left(\frac{\eta}{2-2\eta}\right)}{2\sqrt{\pi}\Gamma\left(\frac{1}{2-2\eta}\right)}\right]^\eta \times \exp\left\{-\int_0^\infty \frac{dt}{t}\left(\frac{\sinh(\eta t)}{\sinh(t)\cosh((1-\eta)t)} - \eta e^{-2t}\right)\right\}. \quad (28)$$

The plot is shown in Fig. 1. There is singularity in function F for η near 1:

$$F \sim (1-\eta)^{-1/2} \quad \text{when} \quad \eta \to 1-0 \quad (29)$$

Special case $\eta=1$ corresponds to *XXX* antiferromagnet.

In Appendix A, we evaluated concurrence before the measurement. It vanishes at finite distance, see Eq. (A32).

IV. *XXX* ANTIFERROMAGNET IN A MAGNETIC FIELD

Let us come back to *XXX* model,

$$H^0_{XXX} = \sum_m \sigma_x^{(m)}\sigma_x^{(m+1)} + \sigma_y^{(m)}\sigma_y^{(m+1)} + \sigma_z^{(m)}\sigma_z^{(m+1)}. \quad (30)$$

But now let us add magnetic field

$$\mathbf{H}^h_{XXX} = H^0_{XXX} - \sum_m h\sigma_z^{(m)}. \tag{31}$$

This introduce anisotropy in a different way. In small magnetic field $h \to 0$, small magnetization develops: $\sigma_z = h/\pi^2$. For stronger magnetic field, magnetization increases. As magnetic field approaches its critical value $h_c = 4$, magnetization approaches 1 (ferromagnetic state with all spins up):

$$\sigma_z = 1 - \frac{2}{\pi}\sqrt{h_c - h}, \quad h \to h_c - 0. \tag{32}$$

Exact expression for magnetization σ_z at arbitrary value of magnetic field is given on pp. 70–71 of [39]. Averages of other spin components over ground state are zero: $\sigma_x = \sigma_y = 0$.

In this section, we are considering moderate magnetic field $0 \leqslant h \leqslant h_c$. Asymptotic of correlation functions at large distances can be described as follows:

$$\langle\langle \phi | \sigma_z^{(i)} \sigma_z^{(j)} | \phi \rangle\rangle = A_1 \frac{1}{(i-j)^2} + A_2 \frac{\cos\{\pi(1-\sigma_z)|i-j|\}}{|i-j|^\theta}. \tag{33}$$

Here double angular brackets on the left-hand side mean that we subtracted σ_z^2, see (4). The coefficients A_1 and A_2 depend on magnetic field. For small magnetic field, critical index θ is close to 1:

$$\theta = 1 + [2\ln(h_x/h)]^{-1} \quad h \to 0; \quad h_x = \sqrt{\frac{8\pi^3}{e}} \tag{34}$$

and for the values of magnetic field close to critical point, θ is close to 2:

$$\theta = 2\left(1 - \frac{1}{\pi}\sqrt{h_c - h}\right), \quad h \to h_c; h \leqslant h_c = 4. \tag{35}$$

In Appendix B we discuss the dependence of θ on magnetic field for intermediate fields. Figure 4 for $\eta = 1$ shows that θ is a monotonic function of the magnetic field. Asymptotic of other correlation functions are

$$\langle \phi | \sigma_x^{(i)} \sigma_x^{(j)} | \phi \rangle = \langle \phi | \sigma_y^{(i)} \sigma_y^{(j)} | \phi \rangle = A(h)|i-j|^{-1/\theta}. \tag{36}$$

Coefficient $A(h)$ vanishes as magnetic field approaches the critical value. Exact formula for θ at any value of magnetic field can be found on pages 73–76 of (Ref. [39] and in Ref. [31]. It shows that $1/2 \leqslant 1/\theta \leqslant 1 \leqslant \theta \leqslant 2$. This means that the lower bound of LE is dominated by σ_x correlations again

$$E_{ij} \geqslant A(h)|i-j|^{-1/\theta}. \tag{37}$$

Now let us discuss the upper bound (3) of LE. Because of translational invariance we have

$$s_+^{ij} = (1 + \langle \phi | \sigma_z^{(i)} \sigma_z^{(j)} | \phi \rangle)^2 - 4\sigma_z^2,$$

$$s_-^{ij} = (1 - \langle \phi | \sigma_z^{(i)} \sigma_z^{(j)} | \phi \rangle)^2. \tag{38}$$

At large space separations $|i-j| \to \infty$, correlations can be simplified $\langle \phi | \sigma_z^{(i)} \sigma_z^{(j)} | \phi \rangle \to \sigma_z^2$. This means that both $s_\pm^{ij}$ approach $(1-\sigma_z^2)^2$. Finally the bounds for LE for large $|i-j|$ are

$$A(h)|i-j|^{-1/\theta} \leqslant E_{ij} < 1 - \sigma_z^2. \tag{39}$$

So magnetic field increases lower bound and deceases upper bound. When magnetic fields are close to the critical value, the bounds become

$$A(h)|i-j|^{-1/2} \leqslant E_{ij} < \frac{4}{\pi}\sqrt{h_c - h}. \tag{40}$$

In Appendix A we evaluated concurrence before the measurement. It vanishes at finite distance, see Eq. (A39).

In the most general case of *XXZ* magnetic field correlations can be described by similar formulas, but parameters h_c, σ_z, θ are different. We shall elaborate in the next section.

V. *XXZ* ANTIFERROMAGNET IN A MAGNETIC FIELD

Let us add interaction with a magnetic field to *XXZ* spin chain:

$$\mathbf{H}^h_{XXZ} = H^0_{XXZ} - \sum_m h\sigma_z^{(m)}. \tag{41}$$

Small magnetic field leads to a small magnetization $\sigma_z = \chi h$. The magnetic susceptibility χ is

$$\chi = \frac{1-\eta}{\pi\eta \sin \pi\eta}. \tag{42}$$

Here we used parameter η related to anisotropy $\Delta = \cos \pi\eta$. The dependence of χ on η is illustrated in Fig. 2. Let us discuss the plot. The meaning of a singularity at $\eta = 0$ is the following: The case $\eta = 0$ corresponds to ferromagnetic *XXX*. At zero magnetic field it has spontaneous magnetization pointed in an arbitrary direction. Weak magnetic field will align spins to the direction of the magnetic field. This makes susceptibility infinite. As η approaches 1, susceptibility approaches $1/\pi^2$ (antiferromagnetic *XXX* case).

For stronger magnetic field, magnetization increases. As magnetic field approaches its critical value $h_c = 2(1-\Delta)$, magnetization approaches 1:

$$\sigma_z = 1 - \frac{2}{\pi}\sqrt{h_c - h}, \quad h \to h_c - 0. \tag{43}$$

Averages of other spin components over ground state are zero: $\sigma_x = \sigma_y = 0$. Here we are considering moderate magnetic field $0 \leqslant h \leqslant h_c$. Asymptotic of correlation functions at large distances can be described by the formulas similar to *XXX* in a magnetic field case see (33) and (36), but critical index θ is different. A formula for θ depends on anisotropy $\Delta = \cos \pi\eta$. Let us first discuss small magnetic field $h \to 0$. Critical index is quadratic in magnetic field for $0 \leqslant \eta \leqslant 2/3$:

$$\theta = \frac{1}{\eta}(1 + \alpha_1 h^2). \tag{44}$$

The coefficient

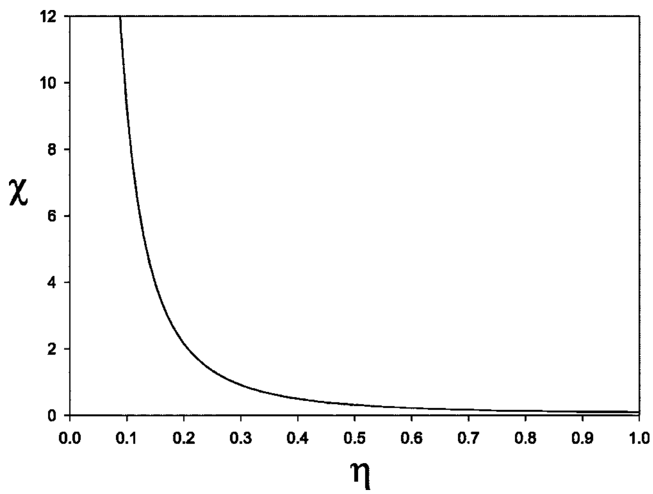

FIG. 2. χ (Eq. (42)) vs η (Eq. (23)).

$$\alpha_1 = \frac{(1-\eta)^2}{4\pi\eta \tan\left(\frac{\pi\eta}{2(1-\eta)}\right)\sin^2\pi\eta} \tag{45}$$

shows singularity at points $\eta=0$ (ferromagnetic *XXX*) and $\eta=2/3$ [$\Delta=-1/2$ case]:

$$\alpha_1 \sim \frac{1}{\pi^4}\frac{1}{\eta^4} \quad \text{for} \quad \eta \to 0+0. \tag{46}$$

$$\alpha_1 \sim \frac{1}{81\pi^2}\frac{1}{(\eta-2/3)} \quad \text{for} \quad \eta \to \left(\frac{2}{3}\right)-0. \tag{47}$$

The nature of dependence of the coefficient α_1 is illustrated in Fig. 3. In case $2/3 \leqslant \eta \leqslant 1$ small h behavior is more complicated:

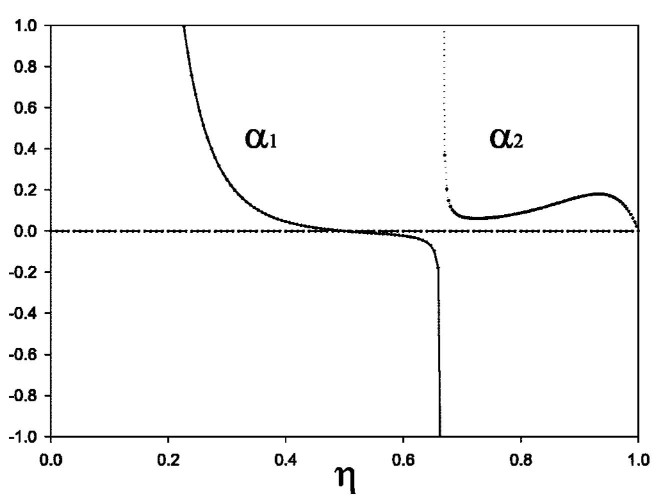

FIG. 3. α_1 (Eq. (45)), α_2 (Eq. (49)) vs η (Eq. (23)).

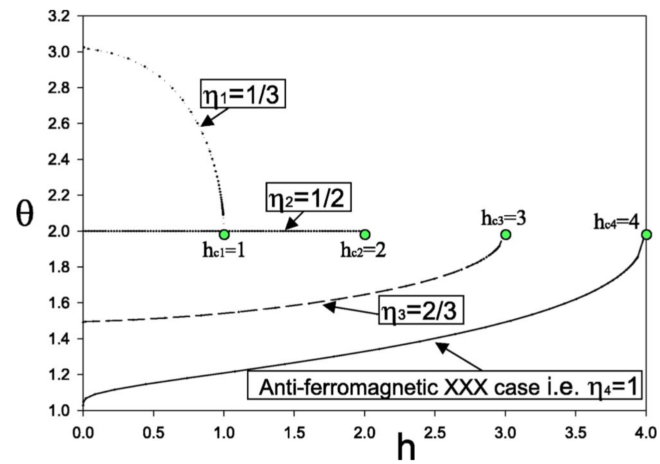

FIG. 4. Critical exponent θ (Eqs. (33) and (36)) vs magnetic field h for different values of anisotropy η.

$$\theta = \frac{1}{\eta}(1+\alpha_2 h^{4(\eta^{-1}-1)}). \tag{48}$$

Notice that the power of magnetic field changes monotonically from 2 at $\eta=2/3$ to 0 at $\eta=1$. An expression for the coefficient α_2 is more complicated:

$$\alpha_2 = 2\eta e^{\frac{2\beta}{\eta}} h_0^{4(1-\eta^{-1})} \tan\left(\frac{\pi}{\eta}\right)\frac{\Gamma^2\left(1+\frac{1}{\eta}\right)}{\Gamma^2\left(\frac{1}{2}+\frac{1}{\eta}\right)}. \tag{49}$$

Here

$$\beta = (1-\eta)\ln(1-\eta) + \eta \ln \eta \tag{50}$$

and

$$h_0 = \frac{4\eta\sqrt{\pi}\sin \pi\eta}{(1-\eta)}\exp\left(\frac{\beta}{2(1-\eta)}\right)\frac{\Gamma\left(\frac{3-2\eta}{2(1-\eta)}\right)}{\Gamma\left(\frac{2-\eta}{2(1-\eta)}\right)}. \tag{51}$$

$\alpha_2(\eta)$ shows singularity at point $\eta=2/3$,

$$\alpha_2 \sim \frac{1}{81\pi^2}\frac{1}{(\eta-2/3)} \quad \text{for} \quad \eta \to \left(\frac{2}{3}\right)+0. \tag{52}$$

The nature of dependence of α_2 on η is illustrated in Fig. 3. We see that at $\eta=2/3$ critical index θ strongly depends on weak magnetic field. It also depends strongly on weak magnetic field for $\eta=1$, which is antiferromagnetic *XXX* case.

For magnetic field close to critical, the index θ approaches 2:

$$\theta = 2 + \frac{4\sqrt{h_c-h}}{\pi \tan\left(\frac{\pi\eta}{2}\right)\tan \pi\eta}. \tag{53}$$

In Appendix B we discuss the dependence of θ on magnetic field for intermediate fields. Figure 4 shows the dependence of θ on magnetic field for different values of η. Note that the dependence is monotonic.

For *XXZ* in a magnetic field the lower bound of localizable entanglement is also given by σ_x correlations

$$E_{ij} \geqslant \langle \phi | \sigma_x^{(i)} \sigma_x^{(j)} | \phi \rangle. \tag{54}$$

Asymptotic of the σ_x correlations is still given by the formula (36) with θ described in this section.

VI. SUMMARY

In this paper we showed that correlations in spin chains are important not only for condensed mater physics and statistical mechanics but also for quantum information. We considered boundaries for localizable entanglement in the ground state of antiferromagnetic spin chains. We showed that anisotropy raises the localizable entanglement. We also calculated concurrence before the measurement to illustrate that the measurement raises the concurrence.

There are still two open problems left: (i). to prove that localizable entanglement coincide with the lower bound $E_{ij} = \max_\alpha(|Q^{ij}_{\alpha\alpha}|)$, (ii) to calculate localizable entanglement for positive temperature.

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APPENDIX A

In this Appendix, we calculate the concurrence between two marked spins before measurement. We show that the concurrence between ith and jth qubits vanishes at finite distance $|i-j|$ before the measurement. The density matrix ρ of ith and jth spins can be represented as

$$\rho = \frac{1}{4} \sum_{\mu_i} \sum_{\mu_j} (\sigma_{\mu_i}^{(i)} \otimes \sigma_{\mu_j}^{(j)}) \langle \sigma_{\mu_i}^{(i)} \sigma_{\mu_j}^{(j)} \rangle. \tag{A1}$$

To calculate concurrence we need

$$\tilde{\rho} = (\sigma_y \otimes \sigma_y) \rho^* (\sigma_y \otimes \sigma_y). \tag{A2}$$

Here ρ^* is the complex conjugate of ρ. Subindex μ runs though four different values $\mu = 0, x, y, z$. Pauli matrix σ_μ are

$$\sigma_0 = I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \tag{A3}$$

$$\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{A4}$$

Following Wooters [15] we define

$$R = \sqrt{\sqrt{\rho} \tilde{\rho} \sqrt{\rho}}. \tag{A5}$$

We shall denote the eigenvalues of R by λ_k in a decreasing order

$$\lambda_1 \geqslant \lambda_2 \geqslant \lambda_3 \geqslant \lambda_4.$$

Then concurrence (C) can be expressed as

$$C = \max\{0, \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4\}.$$

Let us start with the most general case *XXZ* in a magnetic field:

$$\langle \sigma_x^{(j)} \rangle = \langle \sigma_y^{(j)} \rangle = 0; \quad \langle \sigma_z^{(j)} \rangle = \sigma \quad \text{and} \quad 0 \leqslant \sigma < 1; \tag{A6}$$

$$\langle \sigma_x^{(i)} \sigma_y^{(j)} \rangle = 0; \quad \langle \sigma_x^{(i)} \sigma_z^{(j)} \rangle = \langle \sigma_y^{(i)} \sigma_z^{(j)} \rangle = 0; \tag{A7}$$

$$\langle \sigma_x^{(i)} \sigma_x^{(j)} \rangle = \langle \sigma_y^{(i)} \sigma_y^{(j)} \rangle = g_x(i-j); \tag{A8}$$

$$\langle \sigma_z^{(i)} \sigma_z^{(j)} \rangle = G(i-j) = \sigma^2 + g_z(i-j); \tag{A9}$$

$$0 < |g_z(i-j)| < |g_x(i-j)| < 1 \quad \text{for large} \quad |i-j|. \tag{A10}$$

Hence density matrix ρ for ith and jth qubits (spins) can be expressed as

$$\rho = \frac{1}{4} I \otimes I + \frac{g_x(i-j)}{4} (\sigma_x \otimes \sigma_x + \sigma_y \otimes \sigma_y) + \frac{G(i-j)}{4} \sigma_z \otimes \sigma_z + \frac{\sigma}{4} (I \otimes \sigma_z + \sigma_z \otimes I). \tag{A11}$$

All coefficients σ, $g_x(i-j)$, $G(i-j)$ are real, so

$$\rho^* = \rho, \tag{A12}$$

$$\tilde{\rho} = (\sigma_y \otimes \sigma_y) \rho (\sigma_y \otimes \sigma_y). \tag{A13}$$

The first three terms in Eq. (A11) commute with $\sigma_y \otimes \sigma_y$ and the last term anti-commutes. Let us define

$$\rho_0 = \frac{I \otimes I}{4} + \frac{g_x(i-j)}{4} (\sigma_x \otimes \sigma_x + \sigma_y \otimes \sigma_y) + \frac{G(i-j)}{4} \sigma_z \otimes \sigma_z \tag{A14}$$

and

$$m = \frac{\sigma}{4} (I \otimes \sigma_z + \sigma_z \otimes I). \tag{A15}$$

Notice that $[I \otimes \sigma_z + \sigma_z \otimes I, \sigma_x \otimes \sigma_x + \sigma_y \otimes \sigma_y] = 0$. So we have

$$\rho = \rho_0 + m, \quad \tilde{\rho} = \rho_0 - m, \quad [\rho_0, m] = 0, \tag{A16}$$

$$[\rho, m] = 0, \quad [\tilde{\rho}, m] = 0, \quad [\rho, \tilde{\rho}] = 0. \tag{A17}$$

Now we can simplify the expression for the matrix R:

$$R = \sqrt{\sqrt{\rho} \tilde{\rho} \sqrt{\rho}} = \sqrt{\tilde{\rho} \rho} = \sqrt{\rho_0^2 - m^2}. \tag{A18}$$

Using this representation we can diagonalize R. Corresponding four eigenvalues $\{\lambda_k\}$ are:

$$\left\{\frac{1}{4}\sqrt{(1+G(i-j))^2-4\sigma^2},\frac{1}{4}\sqrt{(1+G(i-j))^2-4\sigma^2},\right.$$
$$\left.\frac{1-G(i-j)}{4}+\frac{g_x(i-j)}{2},\frac{1-G(i-j)}{4}-\frac{g_x(i-j)}{2}\right\} \tag{A19}$$

Now let us consider separately the following special case

I. *XXX model with* $h=0$.

In this case, $\sigma=0$ and

$$G(i-j)=g_x(i-j)=g_z(i-j)=g,$$

The set of eigenvalues of R becomes

$$\{\lambda_k\}=\left\{\frac{1+g}{4},\frac{1+g}{4},\frac{1+g}{4},\frac{1-3g}{4}\right\}. \tag{A20}$$

To get an explicit expression for concurrence we need to consider separately two cases:

A: $g>0$ (for $|i-j|=even$):

$$\lambda_1=\lambda_2=\lambda_3=\frac{1+g}{4},\quad \lambda_4=\frac{1-3g}{4}. \tag{A21}$$

We can calculate the concurrence C,

$$C=\max\left\{0,-\frac{1-g}{2}\right\}=0, \tag{A22}$$

since $|g|<1$.

B: $g<0$ (for $|i-j|=odd$);

$$\lambda_1=\frac{1-3g}{4},\lambda_2=\lambda_3=\lambda_4=\frac{1+g}{4}. \tag{A23}$$

The concurrence

$$C=\max\left\{0,\frac{-3g-1}{4}\right\} \tag{A24}$$

is non-zero only if $g<-\frac{1}{3}$. This happens only for $j=i\pm1$ with

$$g=\langle\sigma_j^z\sigma_{j+1}^z\rangle=\frac{1-4\ \ln2}{3}\approx-0.591. \tag{A25}$$

Hence we have

$$C_{j,j+1}=\ln 2-\tfrac{1}{2}\approx0.193,$$

$$C_{j,j+k}=0\quad\text{if}\quad k>1. \tag{A26}$$

So, concurrence is non-zero only for nearest neighbors (for ground state of *XXX* model without magnetic field). It was first discovered in Ref. [34].

II. *XXZ model at* $h=0$.

In this case $\sigma=0$. At $|i-j|\to\infty$

$$g_x(i-j)>0,\quad g_x(i-j)>|g_z(i-j)| \tag{A27}$$

and both $g_x(i-j)$ and $g_z(i-j)$ decay as a function of the distance $|i-j|$. Eigenvalues of R become

$$\lambda_1=\frac{1-g_z(i-j)}{4}+\frac{g_x(i-j)}{2}; \tag{A28}$$

$$\lambda_2=\lambda_3=\frac{1+g_z(i-j)}{4}; \tag{A29}$$

$$\lambda_4=\frac{1-g_z(i-j)}{4}-\frac{g_x(i-j)}{2}. \tag{A30}$$

Now we can calculate the concurrence:

$$C=\max\left\{0,-\tfrac{1}{2}+g_x(i-j)-\tfrac{1}{2}g_z(i-j)\right\}. \tag{A31}$$

It vanishes at distance larger than $|i-j|_{min}$,

$$\frac{1}{2}\simeq g_x(|i-j|_{min})\simeq\frac{F}{|i-j|_{min}^{\eta}};$$

$$|i-j|_{min}\simeq(2F)^{1/\eta}. \tag{A32}$$

III. *XXX in a magnetic field:*

$$G(i-j)=\sigma^2+g_z(i-j). \tag{A33}$$

For large $|i-j|$ both $g_z(i-j)$ and $g_x(i-j)$ become small. For magnetic field smaller than critical

$$g_z(i-j)\frac{1+\sigma^2}{(1-\sigma^2)^2}\ll1,$$

$$|g_x(i-j)|>|g_z(i-j)|. \tag{A34}$$

Eigenvalues of R in Eq. (A19) become

$$\lambda_1=\frac{1-\sigma^2}{4}-\frac{g_z(i-j)}{4}+\left|\frac{g_x(i-j)}{2}\right|; \tag{A35}$$

$$\lambda_2=\lambda_3=\frac{1-\sigma^2}{4}+\frac{g_z(i-j)}{4}\frac{1+\sigma^2}{1-\sigma^2}; \tag{A36}$$

$$\lambda_4=\frac{1-\sigma^2}{4}-\frac{g_z(i-j)}{4}-\left|\frac{g_x(i-j)}{2}\right|, \tag{A37}$$

and concurrence becomes

$$C=\max\left\{0,|g_x(i-j)|-\frac{1-\sigma^2}{2}-\frac{g_z(i-j)}{2}\frac{1+\sigma^2}{1-\sigma^2}\right\}. \tag{A38}$$

Hence concurrence vanishes at distance lager than $|i-j|_{min}$,

$$\frac{1-\sigma^2}{2}=|g_x(|i-j|_{\mathrm{min}})|=|A(h)||i-j|_{min}^{-1/\theta}$$

$$|i-j|_{min}=\left|\frac{2A(h)}{1-\sigma^2}\right|^{\theta}. \tag{A39}$$

APPENDIX B

In this Appendix, we discuss the dependence of critical exponent θ on the magnetic field h. We follow Ref. [39].

I. Let us start from *XXX model*.

Energy of a magnon $\epsilon(\lambda)$ is defined by a set of equations:

$$\epsilon(\lambda) - \frac{1}{2\pi}\int_{-\Lambda}^{\Lambda} K(\lambda,\mu)\epsilon(\mu)d\mu = \epsilon_0(\lambda), \tag{B1}$$

$$K(\lambda,\mu) = \frac{-2}{1+(\lambda-\mu)^2}, \quad \epsilon_0(\lambda) = 2h - \frac{2}{\frac{1}{4}+\lambda^2}. \tag{B2}$$

With extra condition $\epsilon(\pm\Lambda)=0$. This set of equations determines the dependence of Λ on magnetic field h. Here Λ is a value of a spectral parameter at the Fermi edge. An important object is the fractional charge $Z(\lambda)$:

$$Z(\lambda) - \frac{1}{2\pi}\int_{-\Lambda}^{\Lambda} K(\lambda,\mu)Z(\mu)d\mu = 1. \tag{B3}$$

The critical exponent is equal to

$$\theta = 2Z^2(\Lambda). \tag{B4}$$

For *XXX* model, the critical field $h_c=4$. For large magnetic field $(|h|>h_c)\Lambda=0$. If magnetic field approaches the critical value from below, then

$$\Lambda = \frac{1}{2}\sqrt{h_c-|h|} \quad \text{and} \quad \theta = 2 - \frac{4}{\pi}\Lambda \to 2. \tag{B5}$$

If the magnetic field is small $|h|\to 0$ then

$$\Lambda = \frac{1}{2\pi}\ln\left(\frac{(2\pi)^3}{eh^2}\right) \to \infty \quad \text{and} \quad \theta = 1 + \frac{1}{2\pi\Lambda} \to 1 \tag{B6}$$

II. Now let us discuss *XXZ* model.

In this case we can use the same set of equations (B1) and (B2) with $K(\lambda,\mu)$ and $\epsilon_0(\lambda)$ replaced by

$$K(\lambda,\mu) = \frac{\sin(2\pi\eta)}{\sinh(\lambda-\mu+i\pi\eta)\sinh(\lambda-\mu-i\pi\eta)},$$

$$\epsilon_0(\lambda) = 2h - \frac{2\sin^2(\pi\eta)}{\cosh\left(\lambda+\frac{i\pi\eta}{2}\right)\cosh\left(\lambda-\frac{i\pi\eta}{2}\right)}. \tag{B7}$$

For small magnetic field

$$\Lambda = (1-\eta)\ln\left(\frac{h_0}{h}\right) \to \infty \quad \text{when} \quad h \to 0 \tag{B8}$$

Here h_0 is given by (51).

But for magnetic field close to critical:

$$\Lambda = \frac{\sqrt{h_c-|h|}}{2\tan\left(\frac{\pi\eta}{2}\right)} \to 0 \quad \text{when} \quad h \to \pm h_c. \tag{B9}$$

The critical value of the magnetic field is

$$h_c = 2(1-\Delta) = 2(1-\cos(\pi\eta)). \tag{B10}$$

For general magnetic field h, we solved these equations numerically and found that both $\Lambda(h)$ and $\theta(h)$ are monotonic functions of h. The numerical solution for $\theta(h)$ was shown in Fig. 4.

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