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LETTER TO THE EDITOR

A new correlator in quantum spin chains

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Abstract

We propose a new correlator in one-dimensional quantum spin chains, the *s*-emptiness formation probability (*s*-EFP). This is a generalization of the emptiness formation probability (EFP), which is the probability that the first *n* spins of the chain are all aligned downwards. In the *s*-EFP we let the spins in question be separated by *s* sites. The usual EFP corresponds to the special case when $s = 1$. Taking $s > 1$ allows us to quantify non-local correlations. We express the *s*-EFP for the anisotropic XY model in a transverse magnetic field, a system with both critical and non-critical regimes, in terms of a Toeplitz determinant. For the isotropic XY model we find that the magnetic field induces an interesting length scale.

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1. Introduction

The emptiness formation probability (EFP) is defined for a one-dimensional spin-1/2 chain to be the probability of formation of a ferromagnetic string [1, 2], i.e. the probability that the first *n* spins of the chain are all aligned downwards,

$$P(n) = Z^{-1} \operatorname{Tr}\{e^{-H/k_B T} F\}, \tag{1}$$

where H is the Hamiltonian of the system, $Z = \operatorname{Tr}\{e^{-H/k_B T}\}$ is the partition function and

$$F = \prod_{j=0}^{n} \frac{1 - \sigma_j^z}{2}. \tag{2}$$

Here σ_j^z is the usual Pauli spin matrix and j labels the sites on the chain. At zero temperature the EFP is given by

$$P(n) = \langle 0|F|0 \rangle, \tag{3}$$

where $|0\rangle$ denotes the ground state of the system. This fundamental correlator has been the subject of a good deal of recent interest [3–8]. It usually cannot be calculated exactly, but a number of results have been obtained regarding its asymptotic behaviour as $n \to \infty$.

In this letter we propose a new correlator in one-dimensional quantum spin chains: the *s*-emptiness formation probability (*s*-EFP). This is a generalization of the usual EFP. What we consider is the probability of finding *n* equally spaced sites aligned downward, for a given spacing *s*. Specifically, the *s*-EFP is defined as

$$P_s(n) = \langle 0 | \prod_{j=0}^{n} \frac{1 - \sigma_{sj}^z}{2} | 0 \rangle. \tag{4}$$

Note that we take the Pauli matrices at the first *n* sites whose labels are multiples of *s*. The EFP thus corresponds to the particular case when $s = 1$. Since (4) is not restricted to adjacent spins the *s*-EFP contains non-local information that is not available through the EFP. For the anisotropic XY model we shall derive its asymptotic form as $n \to \infty$ using the theory of Toeplitz determinants. For simplicity we take the temperature to be zero, but an extension to finite temperature is straightforward.

2. EFP and *s*-EFP for the XY model

Abanov and Franchini have recently considered the EFP for the anisotropic XY model in a transverse magnetic field *h* [8]. They used the theory of Toeplitz determinants and extensions of what is generally known as the Fisher–Hartwig conjecture [9, 10] to obtain the asymptotic ($n \to \infty$) behaviour of $P(n)$. The XY Hamiltonian is

$$H = \sum_{j=0}^{N-1} \left(\frac{1+\gamma}{2} \sigma_j^x \sigma_{j+1}^x + \frac{1-\gamma}{2} \sigma_j^y \sigma_{j+1}^y \right) - h \sum_{j=0}^{N-1} \sigma_j^z, \tag{5}$$

and it is critical along the lines $\gamma = 0$, $|h| < 1$ and $h = \pm 1$, i.e., quantum correlations decay algebraically when the parameters are on these lines and exponentially when they lie away from them [11, 12]. The EFP can in this case be written as

$$P(n) = |\det S_n|, \tag{6}$$

where S_n is an $n \times n$ Toeplitz matrix whose elements are

$$(S_n)_{jk} = \frac{1}{2\pi} \int_0^{2\pi} e^{i(j-k)\theta} \sigma(\theta) \, d\theta. \tag{7}$$

The function $\sigma(\theta)$ is called the symbol of the matrix S_n, and is given by

$$\sigma(\theta) = \frac{1}{2} + \frac{1}{2} \frac{\cos\theta - h + i\gamma \sin\theta}{\sqrt{(\cos\theta - h)^2 + \gamma^2 \sin^2\theta}}. \tag{8}$$

Abanov and Franchini obtained the asymptotic form of the determinant (6) in all regions of the γ–h phase diagram. Their results are as follows [8]: for $1 > h \neq -1$, $P(n) \sim E \, e^{-n\beta}$; for $h > 1$, the previous result is multiplied by $[1 + (-1)^n A]$; on the critical lines $h = \pm 1$, $P(n) \sim En^{-1/16}[1 + (-h)^n A/\sqrt{n}]e^{-n\beta}$; and on the critical line $\gamma = 0$, $|h| < 1$, $P(n) \sim En^{-1/4} e^{-n^2\alpha}$, i.e. the decay is Gaussian. Explicit formulae were obtained for E, A, α and β as functions of γ and h. The latter, for example, is given by

$$\beta = -\frac{1}{2\pi} \int_0^{2\pi} d\theta \, \log|\sigma(\theta)|. \tag{9}$$

For this system the *s*-EFP corresponds simply to

$$P_s(n) = |\det S_n(s)|, \tag{10}$$

where $S_n(s)$ is obtained from S_n by removing the rows and columns whose labels are not multiples of s. Its matrix elements are

$$(S_n(s))_{jk} = \frac{1}{2\pi} \int_0^{2\pi} e^{is(j-k)\theta} \sigma(\theta)\, d\theta. \tag{11}$$

This is in Toeplitz form, but $\sigma(\theta)$ is no longer the symbol. To determine the symbol we must find the function σ_s that satisfies

$$\int_0^{2\pi} \sigma(\alpha)\, e^{-isn\alpha}\, d\alpha = \int_0^{2\pi} \sigma_s(\alpha)\, e^{-in\alpha}\, d\alpha. \tag{12}$$

Multiplying (12) by $e^{in\theta}$ with $0 \leqslant \theta < 2\pi$, summing over n and using the Poisson summation formula, we arrive at

$$\sigma_s(\theta) = \frac{1}{s} \sum_{n=0}^{s-1} \sigma\left(\frac{\theta}{s} + \frac{2n\pi}{s}\right). \tag{13}$$

The value of σ_s at the point θ is therefore obtained as the average value of the original symbol σ over the s vertices of a regular polygon. Hence the s-emptiness formation probability of the XY model (5) can also be computed as a Toeplitz determinant.

Given the parameters γ and h, the numerical calculation of the average (13) is a trivial task. Exact analytical results, on the other hand, are only available for particular cases. One of these cases is the isotropic XY model, which we analyse in the next section.

3. The isotropic XY model

As a simple application, let us consider the isotropic XY model, for which $\gamma = 0$. In the non-critical regime $|h| > 1$ the ground state is always a ferromagnet, i.e., the spins are all aligned up if $h > 1$, and all aligned down if $h < -1$. Therefore $P(n)$ vanishes in the first case and is unity in the second. Since the chain is translation-invariant, $P_s(n)$ is the same as $P(n)$ for any choice of s.

The critical regime $|h| < 1$ is of course much more interesting. The symbol (8) reduces to

$$\sigma(\theta) = \begin{cases} 1 & \text{if } -k \leqslant \theta < k, \\ 0 & \text{otherwise,} \end{cases} \tag{14}$$

where k is related to the magnetic field by

$$h = \cos k. \tag{15}$$

Applying Widom's theorem [10] to the resulting Toeplitz determinant, one concludes that as $n \to \infty$ the EFP behaves like $P(n) \sim E n^{-1/4} e^{n^2\alpha}$, where E and α are explicitly determined constants. In order to obtain the s-EFP we must compute the average (13), which in this case can be done explicitly. The result is a piecewise constant and even function, with jumps at the critical points $\pm\theta^*$ given by

$$[0, \pi) \ni \theta^* = \min\{\alpha, 2\pi - \alpha\}, \qquad \alpha = sk \bmod 2\pi, \tag{16}$$

and values

$$\sigma_s(\theta) = \frac{1}{s}\left(1 + 2\left[\frac{sk}{2\pi}\right]\right) + \begin{cases} 0 & \text{if } |\theta| < \theta^*, \\ \epsilon/s & \text{otherwise,} \end{cases} \tag{17}$$

where the brackets $[\cdot]$ denote the integer part and

$$\epsilon = \text{sign}\{\alpha - \pi\}. \tag{18}$$

If $s < \pi/k$ we have $\sigma_s(0) = 1/s$ and $\sigma_s(\pi) = 0$. In this case we get simply $P_s(n) = s^{-n} P(n)$, so the s-EFP decays much faster than the EFP, combining the original Gaussian decay with an additional exponential term that depends on the spacing. On the other hand, if $s > \pi/k$ then the function $\sigma_s(\theta)$ is never zero, and instead of applying Widom's theorem we should apply the Fisher–Hartwig conjecture [9]. In that case the decay is no longer Gaussian, but becomes an exponential with a power-law prefactor,

$$P_s(n) \sim E n^{-\xi} \, e^{-\beta n}. \tag{19}$$

The constant E can be obtained from the Fisher–Hartwig formula and the other quantities are

$$\beta(s) = -\frac{1}{\pi}[\theta^* \ln(\sigma_s(0)) + (\pi - \theta^*) \ln(\sigma_s(\pi))] \tag{20}$$

and

$$\xi = \frac{1}{4\pi^2} \ln^2(\sigma_s(\pi)/\sigma_s(0)). \tag{21}$$

Interestingly, the decay of $P_s(n)$ therefore shows a clear transition at the magnetic-field-dependent value $s = \pi/k$, changing from Gaussian to exponential. In particular, for large spacings we see that both $\sigma_s(0)$ and $\sigma_s(\pi)$ tend to k/π. Hence in this limit there is no power-law prefactor and the exponent saturates:

$$\lim_{s \to \infty} \beta(s) = \ln(\pi/k). \tag{22}$$

It is important to observe that expression (20) for the exponent $\beta(s)$ is continuous when we consider s as a real number, despite the discontinuities that appear in (17). The function $\sigma_s(0)$ is discontinuous whenever $sk = 2n\pi$, but at those points θ^* vanishes and hence $\beta(s)$ remains unaffected. The same is true for the jumps in the function $\sigma_s(\pi)$, which occur at $sk = (2n+1)\pi$ (due to the variable ϵ), because then we have $\theta^* = \pi$. The derivative $\beta'(s)$, on the other hand, is discontinuous: at the special points $sk = n\pi$ the function $\beta(s)$ has a local minimum with a cusp form. Remarkably, for a fixed k its value at the minimum is independent of n, and is actually equal to its $s \to \infty$ limit,

$$\beta(n\pi/k) = \ln(\pi/k). \tag{23}$$

In figure 1 we plot the function $\beta(s)$ for different values of the magnetic field $h = \cos k$. Since, of course, only integer values of s may be realized in the actual chain, we pick values of the form $k = \pi/\ell$ with an integer ℓ. We see that this leads to the appearance of the above mentioned new length scale: $\beta(s)$ attains its minimal value whenever s is a multiple of ℓ. It is worth remarking that Toeplitz determinants have also been used to describe quantum entanglement [13–15], and that a generalization of the usual entanglement geometry, similar to the one proposed here, involving spins that are s sites apart, exhibits behaviour like that of the s-EFP [16].

4. The line $\gamma^2 + h^2 = 1$

In the phase diagram of the XY model the line $\gamma^2 + h^2 = 1$, which Franchini and Abanov call Γ_E, is special. Along it the ground state is completely disentangled [17], i.e., it is given by

$$|0\rangle_{\Gamma_E} = \prod_j [\cos(\vartheta/2)|\uparrow\rangle_j + (-1)^j \sin(\vartheta/2)|\downarrow\rangle_j], \tag{24}$$
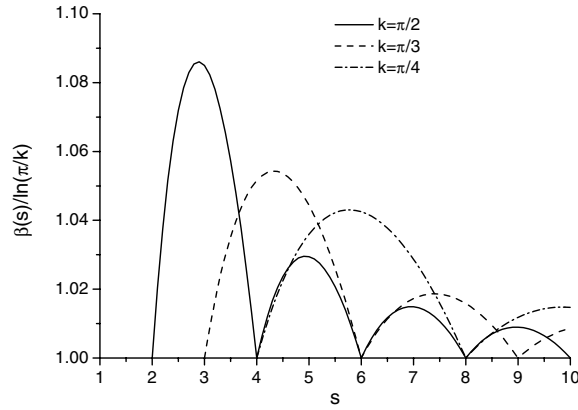
Figure 1. The renormalized exponent $\beta(s)/\ln(\pi/k)$, defined in (20), for some values of the magnetic field $h = \cos k$. We see that for $k = \pi/\ell$ there exists a typical length scale for the spacing s: the exponent is minimal for $s = n\ell$, and its value is equal to its asymptotic value. Notice that the exponent $\beta(s)$ is not defined for $s < \ell$ because in this regime the decay is Gaussian. The point $s = \ell$ marks a crossover in the behaviour of $P_s(n)$.

where $|\!\uparrow\rangle_j$ and $|\!\downarrow\rangle_j$ denote spin-up and spin-down states respectively at the site j, and the parameter ϑ is such that

$$\cos\vartheta = \sqrt{\frac{1-\gamma}{1+\gamma}}. \tag{25}$$

Let us consider, for simplicity of notation, only the case $h > 0$. Then the symbol (8) is given by

$$\sigma_{\Gamma_E}(\theta) = \frac{1}{2}\left(1 + \frac{z - \cos\vartheta}{1 - z\cos\vartheta}\right), \tag{26}$$

where $z = e^{i\theta}$. The average (13) becomes

$$\left(\sigma_{\Gamma_E}\right)_s(\theta) = \frac{1 - \cos\vartheta}{2} + \frac{\sin^2\vartheta}{2}\frac{z\cos^{s-1}\vartheta}{1 - z\cos^s\vartheta}, \tag{27}$$

and its modulus is

$$\left|\left(\sigma_{\Gamma_E}\right)_s(\theta)\right| = \frac{1 - \cos\vartheta}{2}\left|\frac{1 + z\cos^{s-1}\vartheta}{1 - z\cos^s\vartheta}\right|. \tag{28}$$

As expected, the s-emptiness formation probability in this case is independent of s, because the exponent β is given by

$$\beta = -\log\left(\frac{1 - \cos\vartheta}{2}\right), \tag{29}$$

and we thus have

$$P_s(n) = \left(\frac{1 - \cos\vartheta}{2}\right)^n = \sin^{2n}(\vartheta/2), \tag{30}$$

which is in fact an exact result.

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