Temperature dependent spatial oscillations in the correlations of the XXZ spin chain

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We study the correlation $\langle \sigma_0^z \sigma_n^z \rangle$ for the XXZ chain in the massless attractive (ferromagnetic) region at positive temperatures by means of a numerical study of the quantum transfer matrix. We find that there is a range of temperatures by means of a numerical study of the quantum transfer matrix. We find that there is a range of temperature where the behavior of the correlation for large separations is oscillatory with an incommensurate period which depends on temperature.

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I. INTRODUCTION

Recently we [1, 2] have studied the finite temperature spin correlation function

$$S^z(n; T, \Delta) = \text{Tr} \sigma_0^z \sigma_n^z e^{-H/kT}/\text{Tr} e^{-H/kT}$$

(1)

for the spin 1/2 XXZ spin chain [3] - [4].

$$H = \frac{1}{2} \sum_{j=0}^{L-1} (\sigma_j^x \sigma_{j+1}^x + \sigma_j^y \sigma_{j+1}^y + \Delta \sigma_j^z \sigma_{j+1}^z).$$

(2)

In [1] we made a finite size study of $S^z(n; T, \Delta)$ for chains of size up to $L = 18$ and found that for $-1 < \Delta < 0$ there is a range of temperature where the correlation function changes sign as a function of $n$ starting from negative values for $n = 1$. For $T$ sufficiently low the correlations for $-1 < \Delta < 0$ are negative for all $n$ whereas for sufficiently large $T$ the correlations are positive for all $n$. We referred to this change in sign as a quantum classical crossover.

In both [1] and [2] we discussed the representation of this correlation function for the chain with $L \to \infty$ in terms of an expansion in terms of eigenvalues and eigenvectors of the quantum transfer matrix [3], [5]:

$$S^z(n; T, \Delta) = \sum_j A_j (\lambda_j/\lambda_0)^{n-1}$$

(3)

where $\lambda_0$ is the maximum eigenvalue of the quantum transfer matrix and is directly related to the free energy per lattice site by

$$f = -kT \ln \lambda_0 + \Delta/2$$

(4)

This quantum transfer matrix is defined as the limit $N \to \infty$ of a matrix of dimension $2^N$ where $N$, which is even, is the “Trotter number” (and is not to be confused with the chain length $L$ which is taken to infinity.) We have numerically studied this expansion for values of $N$ as large as 16 and have found several features of the correlations which have not previously been seen which substantially expands our understanding of the phenomena of quantum-classical cross over.

From our study we find that as the temperature increases from zero the following phenomena occur:

1. There is a temperature $T_V(\Delta)$ below which all amplitudes $A_j$ are negative and at which temperature all $A_j$ vanish. There is no other temperature at which any $A_j$ vanishes. For $T < T_V(\Delta)$ all eigenvalues are real. This temperature vanishes as $1/N$ as $N \to \infty$. We will refer to $T_V(\Delta)$ as the universal vanishing temperature.

2. There is a temperature $T_C(\Delta) > T_V(\Delta)$ above which real eigenvalues collide and become complex conjugate pairs. At the temperatures where the collision of the eigenvalues occurs the amplitudes $A_j$ diverge as a square root. In the limit $N \to \infty$ we have $T_C(\Delta) \to T_V(\Delta)$.

3. There is a temperature $T_L(\Delta) > T_C(\Delta)$ where the eigenvalue in [4] with the largest magnitude becomes complex. As $N \to \infty$ $T_L(\Delta)$ approaches a nonzero limiting value from above. We refer to $T_L(\Delta)$ as the lower crossover temperature.

4. There is a temperature $T_U(\Delta) > T_L(\Delta)$ where the eigenvalue in [4] with the largest magnitude becomes real and the corresponding amplitude is positive. At $T_U(\Delta)$ eigenvalues with different quantum numbers cross. As $N \to \infty$ $T_U(\Delta)$ approaches its limiting value from below. We refer to $T_U(\Delta)$ as the upper crossover temperature.

We conclude that for $T$ between $T_L(\Delta)$ and $T_U(\Delta)$ the correlation $S^z(n; T, \Delta)$ oscillates and changes sign an infinite number of times as $n \to \infty$.

In the remainder of this letter we will present the evidence to support and illustrate these conclusions.
II. THE UNIVERSAL VANISHING TEMPERATURE $T_V(\Delta)$

At $T = 0$ it has been known for some time \[14\] when $n \to \infty$ that for $-1 < \Delta < 0$

$$S^z(n; 0, \Delta) \sim \frac{1}{\pi^2 n^{2/3} + (-1)^n C(\Delta)} n$$

(5)

where $\cos \pi \theta = -\Delta$ and the constant $C(\Delta)$ has recently been conjectured \[11\]. In the very low temperature limit $T \to 0$ and $n \to \infty$ with $n T = \pi r$ fixed where conformal field theory is applicable \[12\]- \[13\] the large $n$ behavior of $S^z(n, T, \Delta)$ is obtained from (4) by the replacement \[14\]

$n \to (\kappa T/2)^{-1} \sin \kappa r/2$ where $\kappa = \pi (1 - \theta)/\sin \pi \theta$.

From our numerical study we find that for sufficiently low temperatures all eigenvalues $\lambda_j$ are real (although not all are positive) and all amplitudes $A_j$ are negative. We illustrate this in table 1 where we show the first 13 eigenvalues and amplitudes in (3) for $\Delta = -0.5, T = .1, N = 12$. We choose $\Delta = -0.5$ only for purposes of illustration. All phenomena discussed in this paper occur generally for $-1 < \Delta < 0$. Here, and in the subsequent tables, we give only the eigenvalues in the subspace which is odd under spin inversion because the matrix elements in the complementary subspace are identically zero. We also give the quantum number $k$ which plays for the quantum transfer matrix the role which momentum plays for the row transfer matrix. We note for $N \equiv 0(\text{mod} 4)$ that $k = 0, \pm 1, \cdots, \pm (N/4 - 1), N/4$ and for $N \equiv 2(\text{mod} 4)$ that $0, \pm 1, \cdots, \pm (N/2 - 1)$. The eigenvalues for $+k$ are degenerate because of reflection symmetry of the quantum transfer matrix.

| $j$ | $|\lambda_j/\lambda_0|$ | $\lambda_j$ phase | $|A_j|$ | $A_j$ phase | $k$ |
|-----|--------------------------|-------------------|--------|-------------|-----|
| 1.2 | 0.5617564                | 0.0               | 2.9966227 \times 10^{-2} | $\pi$ | $\pm 1$ |
| 3   | 0.3954749                | $\pi$             | 5.619120 \times 10^{-3}  | $\pi$ | 0       |
| 4.5 | -0.3346469               | 0.0               | 3.259733 \times 10^{-2}  | $\pi$ | $\pm 2$ |
| 6   | -0.232767                | 0.0               | 4.927463 \times 10^{-2}  | $\pi$ | 3       |
| 7.8 | -0.191818                | $\pi$             | 1.733955 \times 10^{-2}  | $\pi$ | $\pm 2$ |
| 9.10| -0.1833028               | 0.0               | 4.491119 \times 10^{-3}  | $\pi$ | $\pm 1$ |
| 11.12| -0.1764959              | 0.0               | 1.292250 \times 10^{-2}  | $\pi$ | $\pm 1$ |
| 13  | 0.1728539                | 0.0               | 1.158930 \times 10^{-2}  | $\pi$ | 0       |

TABLE I. Eigenvalues below $T_V(\Delta)$. The first 13 eigenvalues $\lambda_j$ and amplitudes $A_j$ for $\Delta = -0.5, T = .16382224$ and $N = 12$. The value of $\lambda_0$ is 10.7928. The column $j$ is the value of $j$ of the corresponding eigenvalue for $T = .1$ in table 1.

The numerically determined values of $T_V(\Delta) = 10.12, 14, 16$ are given in table 6. The $N$ dependence is extremely well fit for $6 \leq N \leq 16$ by $T_V(\Delta, N) = 1.6539/N$ and therefore $T_V(\Delta)$ vanishes as $N \to \infty$. We thus conclude that the data for $T < T_V(\Delta)$ and $N$ finite is not relevant to the genuine quantum system with $N \to \infty$.

III. COMPLEX EIGENVALUES

As the temperature is increased above the universal vanishing temperature $T_V(\Delta)$ we very soon reach a temperature where two real eigenvalues collide and become complex conjugate pairs. This happens first with eigenvalues which are very small. As $T$ increases beyond the temperature of first collision $T_C(\Delta)$ successively larger eigenvalues collide. At each collision the amplitudes diverge however the correlation functions remain finite due to a perfect phase difference of $\pi$ at the point of level collision. At the temperature of collision the relevant exponential decay terms in (3) are replaced by $A_n(\lambda_j/\lambda_0)^{n-1}$. We illustrate the collision of eigenvalues in table 3 where for $\Delta = -0.5$ and $N = 12$ we give the first 13 eigenvalues and amplitudes at $T = .151493876679$ which is slightly above the collision temperature for the pairs of eigenvalues 4,5 and 6,7. Because the temperature is above collision the eigenvalues and amplitudes of the eigenvalues 4,5,6,7 are complex and all four combinations of the signs of these two phases are to be used. It is clear from the table that the amplitudes are diverging and the change in phase of the amplitude from real to $\pi/2$ suggests that this divergence must be a square root. Further
analysis of the behavior of the amplitudes in the vicinity of the collision shows that this is indeed the correct behavior.

| j   | \(|\lambda_j/\lambda_0|\) | \(\lambda_j\) phase | \(|A_j|\) | \(A_j\) phase | k |
|-----|-----------------|-------------------|---------|----------------|---|
| 1.2 | .4481334        | 0.0               | 4.941102×10^{-3} | π ±1          |   |
| 3   | .2918946        | π                 | 7.509636×10^{-3} | π 0           |   |
| 4-7 | .1909054 ±1.1899×10^{-6} | 4.245×10^{-3} ±1.5708 ±2 |   |
| 8.9 | .1746361        | 0.0               | 5.837584×10^{-3} | 0 ±1          |   |
| 10  | .1741270        | 0.0               | 4.018312×10^{-3} | 0 0           |   |
| 11  | .1561094        | 0.0               | 5.198129×10^{-2} | π 3           |   |
| 12,13 | .1180399     | π                 | 3.785983×10^{-3} | π ±1          |   |

**TABLE III.** A collision of eigenvalues below \(T_L(\Delta)\).

The first 13 eigenvalues \(\lambda_j\) and amplitudes \(A_j\) for \(\Delta = -5, T = 0.151493876679\) and \(N = 12\). The value of \(\lambda_0\) is 8.224613. The order of eigenvalues is the same as in table 2. The phases and the magnitude of \(|A_j|\) for eigenvalues 4-7 have only been determined to four places because of the numerical instabilities resulting from the divergence of \(A_j\).

**IV. THE ONSET OF OSCILLATIONS AT THE LOWER CROSSOVER TEMPERATURE \(T_L(\Delta)\)**

As the temperature is increased further we reach a temperature \(T_L(\Delta)\) where the two eigenvalues with the largest magnitudes collide and produce a complex conjugate pair. These eigenvalues are in the sectors \(k = ±1\).

For \(\Delta = -5\) and \(N = 12\) this occurs slightly below \(T = .22782901\). In table 4 we give the largest 13 eigenvalues at this temperature. The dependence of \(T_L(\Delta)\) on \(\lambda_0\) is given in table 6. This \(N\) dependence is well fit by \(T_L(-5; N) = .4328 - .36/N\) and this has been used to extrapolate to \(N \rightarrow \infty\).

| j   | \(|\lambda_j/\lambda_0|\) | \(\lambda_j\) phase | \(|A_j|\) | \(A_j\) phase | k |
|-----|-----------------|-------------------|---------|----------------|---|
| 1-4 | .2388172 ±1.155×10^{-4} | 1.9078×10^{-2} ±1.570925 ±1 |   |
| 5   | .1815640        | π                 | 7.424416×10^{-3} | π 0           |   |
| 6   | .1799166        | 0.0               | 2.511491×10^{-2} | 0 0           |   |
| 7-10 | .1347183 ±.4576518 | 2.968286×10^{-2} ±2.561349 ±2 |   |
| 11  | .0903745        | 0.0               | 4.730570×10^{-2} | π 3           |   |
| 12,13 | .0614918    | π                 | 2.135921×10^{-3} | π ±1          |   |

**TABLE IV.** Eigenvalues at \(T_L(\Delta)\). The first 13 eigenvalues \(\lambda_j\) and amplitudes \(A_j\) for \(\Delta = -5, T = .22782901\). The value of \(\lambda_0\) is 4.173698.

on \(N\) is given in table 6. This \(N\) dependence is well fit by \(T_L(-5; N) = .2015 + 3.76/N^2\) and this has been used to extrapolate to \(N \rightarrow \infty\).

At the lower crossover temperature the leading asymptotic behavior of the correlation is

\[
S^2(n; T_L(\Delta), \Delta) \sim An(\lambda/\lambda_0)^{n-1}. \tag{6}
\]

As the temperature increases further the leading behavior of the correlation is oscillatory with a wavelength which decreases as \(T\) increases.

**V. THE COMPLETION OF THE CROSSOVER AT THE UPPER CROSSOVER TEMPERATURE \(T_U(\Delta)\)**

In tables 2, 3 and 4 we note that there is a positive eigenvalue with \(k = 0\) which has a positive amplitude. At the lower crossover temperature this eigenvalue does not have the largest magnitude and has \(j = 6\) in table 4 lying below the complex conjugate pairs 1,2 and 3,4 and the negative eigenvalue with the negative amplitude at \(j = 5\). However, as \(T\) is increased from \(T_L(\Delta)\) the magnitude of this eigenvalue increases relative to the magnitude of the leading complex conjugate eigenvalue and at a temperature \(T_U(\Delta)\) the magnitudes of these eigenvalues cross. For \(\Delta = -5\) and \(N = 12\) this occurs very near \(T = .3611\). In table 5 we give the first 13 eigenvalues at a slightly higher temperature where the real eigenvalue has the largest magnitude. Such a crossing without collision is possible because the eigenvalues lie in different sectors \(k\). We call the temperature where this crossing occurs the upper crossover temperature. The dependence of \(T_U(-5)\) on \(N\) is given in table 6. This \(N\) dependence is well fit by \(T_U(-5; N) = .4328 - .36/N\) and this has been used to extrapolate to \(N \rightarrow \infty\).

| j   | \(|\lambda_j/\lambda_0|\) | \(\lambda_j\) phase | \(|A_j|\) | \(A_j\) phase | k |
|-----|-----------------|-------------------|---------|----------------|---|
| 1   | 6               | 1.862180          | 0.0     | 6.113537e-02  | 0  |
| 2-5 | 1-4             | 1.858948 ±.5963864 | 5.134231e-02 ±2.118513 ±1 |   |
| 6-9 | 7-10            | 0.863447 ±.7691693 | 2.144874e-02 ±2.723044 ±2 |   |
| 10  | 5               | 0.989052          | π       | 3.715138e-03  | π  |
| 11  | 1               | 0.428430          | 0.0     | 3.407129e-02  | π  |
| 12-13 | 12-13           | 0.275197          | π       | 6.337585e-04  | π ±1 |

**TABLE V.** Eigenvalues at \(T_U(\Delta)\). The first 13 eigenvalues \(\lambda_j\) and amplitudes \(A_j\) for \(\Delta = -5, T = .3620\) and \(N = 12\). The value of \(\lambda_0\) is 2.679573. The column \(j_5\) is the value of \(j\) of the corresponding eigenvalue in table 4.

For all temperatures above the upper crossover temperature the leading eigenvalue is positive and has a positive amplitude. Consequently for large \(n\) the correlation will be monotonic and positive.

**TABLE VI.** The numerically determined values of the temperatures \(T_V(\Delta), T_L(\Delta)\) and \(T_U(\Delta)\) with \(\Delta = -5\) for various values of \(N\).
VI. CONCLUSIONS

In [1] we found that there is a range of temperatures in which the correlation function $S_z(n; T, \Delta)$ changes sign from negative to positive as $n$ is increased and in [2] we discussed level crossing as a mechanism for this effect. The studies of the eigenvalues of the quantum transfer matrix presented here demonstrate that instead of the single zero seen in the previous finite size studies there is a range of temperatures from $T_L(\Delta)$ to $T_U(\Delta)$ where the correlation function has an oscillatory behavior with a temperature dependent wavelength. This phenomenon has not been seen before in any study of the XXZ chain and can only occur because the non hermitian quantum transfer matrix can have complex eigenvalues. These eigenvalues can be studied analytically by using the Bethe-like equations derived in [3]. However, the necessity of considering complex eigenvalues requires considerations which have not been encountered in previous studies of related Bethe Ansatz equations. As stated previously [2] we believe that the quantum-classical crossover which is seen in the quantum transfer matrix is deeply connected with the bound states at $T = 0$ seen in the spectrum of the Hamiltonian [2]. Analytic investigations of these questions will be pursued elsewhere.

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[1] K. Fabricius and B.M. McCoy, quantum-classical crossover in the spin 1/2 XXZ chain, Phys. Rev. B (in press), cond-mat 9805337.
[2] K. Fabricius, A. Klümper, and B.M. McCoy, Competition of ferromagnetic and antiferromagnetic order in the spin 1/2 XXZ chain at finite temperature, Festschrift for Jim McGuire, cond-mat 9810278.
[3] H.A. Bethe, Z. Phys. 71 (1931) 205.
[4] C.N. Yang and C.P Yang, Phys. Rev. 150 (1966) 321,327; 151 (1966) 258.
[5] M. Suzuki, Phys. Rev. B 31 (1985) 2957.
[6] M. Suzuki and M. Inoue, Prog. Theo. Phys. 78 (1987) 787.
[7] J. Suzuki, Y. Akutsu and M. Wadati, J. Phys. Soc. Japan 59 (1990) 2667.
[8] A. Klümper, Z. Phys. B91 (1993) 507.
[9] A. Luther and I. Peschel, Phys. Rev. B12 (1975) 3908.
[10] H.C. Fogedby, J. Phys. C 11 (1978) 4767.