Exponential asymptotic spin correlations in anisotropic spin-1/2 XY chains at finite temperatures

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The long-time and long-distance asymptotic behavior of the $x$ spin correlations at finite temperature in an anisotropic spin-1/2 XY chain is determined numerically. The decay of the correlations is exponential in both space and time. Similar exponential decay of correlations was already found earlier in the special case of the isotropic model, where analytical expressions for the decay rates could be derived via a mapping to a different model. While no such mapping is known for the anisotropic model, the asymptotic correlations can be very well approximated by a natural generalization of the known analytic results for the isotropic case.

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Spin-1/2 chains are simple quantum many-particle systems which can be defined in terms of a small number of coupling parameters but nevertheless offer a rich variety of interesting static and dynamic phenomena. The simple structure of these models has made possible a large number of links to other models and fields and has fascinated researchers ever since the early days of Ising1 and Bethe.2

The XY chain3,4 is an especially simple example since it can be mapped to a system of noninteracting lattice fermions. Its dynamics are nevertheless nontrivial since single-site spin operators are mapped to strings of Fermi operators and hence two-spin correlation functions correspond to many-fermion correlation functions which may become cumbersome to evaluate analytically.

However, numerical calculations have been important in hinting at the direction where to look for exact analytical results. An early example is the numerical calculation of Sur et al.5 for up to nine spins, suggesting a Gaussian behavior of the infinite temperature $x$ autocorrelation of the isotropic XY chain. That numerical evidence was soon corroborated by independent rigorous proofs for the general XY model from two groups.6-8 Here we report numerical results for the long-time and long-distance asymptotic behavior of the $x$ spin pair correlation functions of anisotropic XY chains. Analytical results for these correlations were derived for the special case of the isotropic model only.9 Our numerical results indicate that the analytic formulas valid in the isotropic case possess natural extensions into the anisotropic regime.

The $S = 1/2$ XY model3,4 is defined by the Hamiltonian

$$H = -\sum_{i=1}^{N-1} \left\{ J \left[ (1 + \gamma) S_i^x S_{i+1}^x + S_i^y S_{i+1}^y \right] + h S_i^z \right\}$$

with anisotropy parameter $0 \leq \gamma \leq 1$. The limiting cases $\gamma = 0$ and $\gamma = 1$ are the isotropic XX and transverse Ising (TI) chains, respectively. The Jordan-Wigner transformation3,4,10

$$S_i^x = a_i^\dagger a_i - \frac{1}{2}, \quad S_i^y = (-1)^{\sum_{k<i} a_k a_k^\dagger} a_i^\dagger, \quad S_i^z = \alpha_i = a_i (-1)^{\sum_{k<i} a_k a_k^\dagger},$$

between the spin-1/2 operators $S_i^x, S_i^y, S_i^z$ at lattice sites $i$ and the creation and annihilation operators $a_i^\dagger, a_i$ of lattice fermions maps the spin Hamiltonian (1) to a Hamiltonian of noninteracting fermions:

$$H = -\sum_{i=1}^{N-1} \left\{ \frac{J}{2} [a_i^\dagger a_{i+1} + a_{i+1}^\dagger a_i + \gamma (a_i^\dagger a_{i+1}^\dagger + a_{i+1} a_i)] \right. $$

$$+ \left. h \left( a_i^\dagger a_i - \frac{1}{2} \right) \right\}.$$  

Note that for $\gamma \neq 0$ the number of fermions is not conserved. From Eqs. (2) and (3), it is evident that the spin correlation functions $\langle S_i^x(t) S_j^x \rangle$ are essentially fermion density correlation functions, while the correlation functions $\langle S_i^y(t) S_j^y \rangle$ are much more complicated when expressed in the fermion representation. The fermionic identity

$$(-1)^{\alpha_i} = (a_i^\dagger + a_i) (a_i^\dagger - a_i)$$

converts the string of signs appearing in Eq. (3) into an expectation value of $2(i + j - 1)$ fermion operators, which may be expressed as a Pfaffian11 by Wick’s theorem. Pfaffians are close relatives of determinants and play a role in several statistical mechanical problems.12 Their numerical evaluation proceeds along similar lines as that of determinants. The numerical calculations of this study were all performed for spin chains with open boundary conditions. Periodic boundary conditions, while desirable from an aesthetic point of view, lead to additional boundary terms in the fermionic model13 which make numerical calculations awkward, if not impossible. Of course, finite-size and boundary effects are a matter of concern in any numerical calculation. They are also a topic of research in their own right and have been studied earlier.11,13,14 In the present study, however, we focus on the asymptotic behavior of bulk spin correlations in the thermodynamic limit. To make sure that open-chain numerical results pertain to that situation, only spins sufficiently far from the boundaries of sufficiently long chains may be considered.

We have checked that the numerical results to be presented below are not subject to finite-size or boundary effects during the time intervals shown.

Several results about exact and asymptotic properties of the dynamic spin correlation functions have been obtained over the years. The asymptotic time dependence of the longitudinal correlation function $\langle S_i^x(t) S_j^x \rangle$ is $\sim t^{-1}$ for all $i$ and $j$ in the bulk of the system at all temperatures.15-17 This can be traced back to the properties of the one-particle density of states.
of the Jordan-Wigner fermions and the fact that $\langle S_i^x(t)S_j^z \rangle$ is related to fermion density correlations. For $i$ and $j$ close to the boundary of a long open chain, the situation is a little more complicated.\textsuperscript{13,14}

Due to its more complicated structure in the fermion representation, the transverse correlation function $\langle S_i^x(t)S_j^z \rangle$ is more sensitive to temperature variations. At infinite temperature, it vanishes for $i \neq j$ and shows Gaussian decay for $i = j$.\textsuperscript{5–8} At zero temperature, that correlation function exhibits an asymptotic power-law decay in both space and time for the isotropic (XX) chain.\textsuperscript{18,19} For finite temperature and in the isotropic case, its et al.\textsuperscript{9} showed that the decay of $\langle S_i^x(t)S_j^z \rangle$ is asymptotically exponential in both space and time; numerical calculations\textsuperscript{11} could be used to assess the range of validity of the exponential asymptotics. Similar exponential behavior at finite temperature was also observed in the TI chain\textsuperscript{20} and in rather general one-dimensional gapless integrable models.\textsuperscript{21}

Asymptotic finite-temperature correlations of the TI chain were also studied in Refs.\textsuperscript{22 and 23}; many interesting results on the zero-temperature correlations of that model were recently obtained by Perk and Au-Yang.\textsuperscript{24}

Before discussing our numerical results, it is useful to recapitulate what is known\textsuperscript{25} about the ground state of the XY Hamiltonian (1) for general anisotropy $\gamma$. Employing a Fourier transform followed by a Bogoliubov transform, $H$ can be brought into diagonal free-fermion form with the single-particle spectrum

$$\varepsilon_k = -\text{sign}(h + J \cos k)\sqrt{(h + J \cos k)^2 + \gamma^2J^2 \sin^2 k}; \quad (-\pi \leq k \leq \pi).$$

The spectrum (for $|h| \leq |J|$) has two branches with negative and positive one-particle energies, respectively, with a gap of size $\Delta \varepsilon = 2|\gamma|\sqrt{J^2 - h^2}$ at the critical wave vector given by $\cos k_c = \frac{h}{J}$. The ground state in the fermionic picture has all negative-energy states occupied and all others empty. The spectral gap closes at the critical field strength $|h| = |J|$ (for arbitrary $\gamma$) and for the isotropic case $\gamma = 0$ and arbitrary $h$ (the XX chain), the case considered by Its et al.\textsuperscript{5} For $\gamma \neq 0$, the ground state exhibits long-range order along the $z$ axis; the magnetization $\langle S_i^z \rangle$ is known analytically.\textsuperscript{25} For $\gamma \neq 0$ and $|h| < |J|$, the ground state also exhibits long-range order in the $xy$ plane:\textsuperscript{26}

$$\lim_{\nu \to \infty} \left| \left| \langle S_i^x S_{i+r}^x \rangle \right| \right|^2 = \frac{\left[ \gamma^2 (1 - (\frac{h}{J})^2) \right]^{\frac{1}{2}}}{2(1 + \gamma)}.\quad (7)$$

At finite temperature, the equilibrium spin correlation functions $\langle S_i^x S_{i+r}^x \rangle$ were shown to decay exponentially with $r$ for all $\alpha = x, y, z$.\textsuperscript{26} For the XX chain, $\gamma = 0$, and subcritical fields, $|h| < |J|$, the finite-temperature asymptotics of $\langle S_i^x(t)S_{i+r}^x(0) \rangle$ were found to be exponential in both space and time.\textsuperscript{5} The derivation of that result proceeded by mapping the correlation function to the solution of a classical nonlinear integrable system related to the nonlinear Schrödinger equation. Despite that intricate derivation, the result can be simply interpreted\textsuperscript{9} in terms of the free energy of quasiparticles with dispersion (6) (for $\gamma = 0$). Generalizing to $\gamma \neq 0$, we conjecture the following asymptotic formula:

$$\langle S_i^x(t)S_{i+r}^x \rangle \propto \begin{cases} \exp(-f(n,0)), & n/v_{0,t} > 1 \\ Ct^\nu \exp(-f(n,t)), & n/v_{0,t} < 1, \end{cases}$$

where

$$f(n,t) = \frac{1}{2\pi} \int_{-\pi}^{\pi} dk \left| n - \int d\varepsilon_k \ln \left| \tanh \frac{\beta\varepsilon_k}{2} \right| \right|,$$\quad (9)

and where

$$\nu = \frac{1}{2\pi} \ln \left| \tanh \left( \frac{\beta\varepsilon_k}{2} \right) \right|,$$\quad (10)

while $k_0$ is determined by $\frac{d^2}{dk} \varepsilon_k = \frac{\nu}{\beta}$. Furthermore,

$$v_0 = \max_{|k| \leq \pi} \left| \frac{d\varepsilon_k}{dk} \right|$$

is the maximum value of the group velocity at which the fermionic quasiparticles move. In the space-like region, $n > v_{0,t}$, the correlation is constant and equal to its stationary value. This is due to the fact that the two spins at distance $n$ have not been able to communicate with each other yet. Only later can the fermionic quasiparticles of energy $\varepsilon_k$ transfer any information at group velocity $\frac{d\varepsilon_k}{dk}$ between the two spins. For zero magnetic field, $h = 0$, the maximum velocity $v_0$ turns out\textsuperscript{27} to be

$$v_0 = (1 - \gamma)J;$$

(12)

for nonzero field, there is no simple closed expression for $v_0$, but numerical evaluation is simple.

The crossover between space-like and time-like regions is illustrated in Fig. 1. In that figure, we show a logarithmic plot of $\left| \left| \langle S_i^x(t)S_{i+r}^x \rangle \right| \right|^2$ for $n = 4, 9, 14, 19$ at temperature $T/J = 2$ and $T/J = 30$.

![FIG. 1. (Main plot) Spin pair correlation function $\langle S_i^x(t)S_{i+r}^x \rangle$ in the bulk regime of the anisotropic XY chain, $\gamma = 0.3$, without external field, $h = 0$, at $T/J = 2$, for $j = 49$ and $i = 30, 35, 40, 45$ (solid lines, bottom to top) in an open chain with $N = 100$ spins. Plotted is the logarithm of $\left| \left| \langle S_i^x(t)S_{i+r}^x \rangle \right| \right|^2$. The marks on the curves denote the boundary between space-like and time-like regions, compare Eq. (8). The inset shows the same function in the same representation, but here the sites are kept fixed ($i = 30, j = 49$) and the temperature is varied ($T/J = 1, 10, 100$, top to bottom). The slopes of the dotted straight-line segments represent the decay rate inferred from the asymptotic expression (8).]
anisotropy $\gamma = 0.3$. We observe that each function is almost perfectly constant up to the time $v_0 t_n = n$, where it bends smoothly into exponential decay with weak superimposed oscillations. The decay time does not show any significant dependence on $n$. The inverse decay time predicted by Eq. (8) for the asymptotic regime of the uppermost curve is given by the slope of the dot-dashed line and matches our data very well. The linear variation with $n$ of the intercepts at $t = 0$ in this logarithmic plot reflects the well-established exponential decay of the equal-time correlation function $\langle S_i^\alpha S_{i+n}^\alpha \rangle \sim \exp(-n/\xi(T))$.

The inset to Fig. 1 shows again the curve $n = 19$ of the main plot along with curves for the same correlation function at different temperatures. Now the crossover between the space-like and the time-like regime occurs roughly at one common value of $Jt$. In the time-like regime, the slope changes from one curve to the next, which reflects the $T$-dependence of the decay time, while the variable intercept in the space-like regime reflects the $T$-dependence of the correlation length.

In Fig. 2, we show results for fixed spatial distance $n = 14$ and fixed temperature $T/J = 10$, for varying anisotropy $\gamma$. For growing $\gamma$, the decay time in the asymptotic regime grows, as does the crossover time between the space-like and time-like regimes. For $\gamma \to 1$, the crossover time diverges since the velocity $v_0$ [Eq. (12)] vanishes. The decay time also diverges as $\gamma \to 1$. This is to be expected, since in the absence of a magnetic field, the model at $\gamma = 1$ (i.e., the transverse Ising chain) does not display any dynamics. The $\gamma$-dependence of the correlation length can be read off from the $t = 0$ intercepts of the curves shown in Fig. 2.

Figure 3 shows the autocorrelation function ($n = 0$) over a longer time interval, demonstrating very clearly how well the conjectured formula (8) fits the numerical results.

The temperature dependence of the autocorrelation function is displayed in Fig. 4 for fixed anisotropy, $\gamma = 0.5$. Two regimes can be clearly distinguished: at short times, the autocorrelation is a Gaussian, crossing over to an exponential behavior at longer times. The crossover time seems to grow roughly logarithmically with temperature, so that at $T \to \infty$, the well-known Gaussian behavior emerges.

The dependence of the spin correlation function on the external field was also observed to follow the asymptotic formula (8) for subcritical ($|h| < |J|$) field values.

To conclude, we have found convincing numerical evidence for exponential decay of the finite-temperature $x$ spin correlations of anisotropic XY chains in both space and time. We
suggest an analytic formula (8) for that exponential decay which fits the numerical data well and which generalizes the known analytical result\(^9\) based on a mapping to a classical nonlinear integrable system. At high temperature, our numerical results connect well to the known\(^6\)–\(^8\) Gaussian infinite-temperature behavior.

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