Thermal entanglement of spins in the Heisenberg model at low temperatures

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Abstract

We calculate the entanglement between two spins in the ferromagnetic Heisenberg chain at low temperatures, and show that when only the ground state and the one-particle states are populated, the entanglement profile is a Gaussian with a characteristic length depending on the temperature and the coupling between spins. The magnetic field only affects the amplitude of the profile and not its characteristic length.

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1 Introduction

Thermal entanglement in many body quantum systems has recently attracted a lot of attention \[1, 2, 3, 4, 5, 6, 7, 8, 9\]. This term is usually used to specify the amount of entanglement which exists between two spins of a multi spin system when the whole system is in a state of thermal equilibrium. There are at least two very good reasons for the interest in this problem. First, it is well known that many body quantum systems may be more correlated than the corresponding classical systems, the excess correlation stemming from a very basic quantum property, namely quantum entanglement \[10, 11, 12\]. Thanks to the progress in the past few years, we have now good measures of entanglement (at least in certain limited cases \[13\]) and it is most natural to quantify this excess correlation or entanglement in many body systems. Once a property like entanglement becomes quantifiable, we can use it as a kind of order parameter and study its behavior when the external parameters of the system change. This will certainly shed light on the nature of quantum phase transition (qualitative change in the nature of the ground state) \[14\]. The second reason is that one dimensional arrays of spins, are a natural candidate for storing quantum information \[15, 16\]. Entanglement is a valuable resource for implementation of any kind of quantum algorithm and quantum information protocol \[17, 18\] and one needs to find the amount of entanglement which exists between spins or qubits and the ways to control it, when the array is in thermal equilibrium.

A prototype of a many body system is the isotropic Heisenberg spin chain whose hamiltonian is as follows:

$$ H = -J \sum_{l=0}^{N-1} \vec{\sigma}_l \cdot \vec{\sigma}_{l+1} + \mu B \sum_{l=0}^{N-1} \sigma^z_l. $$

Here $\sigma^a_l$, where $(a = x, y$ or $z)$ is a spin (Pauli) operator acting only on site $l$ and periodic boundary conditions are assumed.

In this context and to our knowledge, up to now the following studies have been made. Nielsen \[3\] has studied the entanglement of a two-spin system at finite temperature interacting via the Heisenberg interaction. Wang \[5, 6\] and Rigolin \[19\] have also studied the effect of anisotropy on the thermal entanglement in a two spin system. Arnesen, Bose and Vedral have numerically studied the variation of two spin entanglement with temperature and magnetic field in a few-spin isotropic Heisenberg chain \[1\] and Gunlycke et al. \[2\] have studied the same problem in an Ising model in a transverse field where they have observed a kind of quantum phase transition at zero temperature when the entanglement suddenly shows up even with an infinitesimal transverse magnetic field. O’Connor and Wootters \[20\], have calculated the maximum possible entanglement between nearest neighbors in a translationally invariant state and have shown that the ground state of the antiferromagnetic Heisenberg chain satisfies this maximum under certain conditions. Osterloh et al \[7\] have shown that quantum phase transitions of a class of spin systems can be characterized by the...
change in the entanglement between the next and next-nearest neighbors. In particular they have shown that near the point of quantum phase transition the nearest and next-nearest neighbor entanglement exhibit logarithmic divergence and universal behavior. A similar study has been done in [9].

Of particular interest to us here is the work of Wang and Zanardi [4] who have shown that in the isotropic Heisenberg model in the absence of magnetic field, the nearest-neighbor entanglement can be related directly to the free energy of the model. Thus by knowing only the eigenvalues and not the eigenstates, one can calculate the entanglement between nearest neighbor spins. In particular they have shown that in an Heisenberg ferromagnet there is no entanglement between nearest neighbors if $B = 0$.

This is a very rare and fortunate situation where one can draw general conclusions about a problem whose solution generally needs a knowledge of the whole spectrum, i.e. the eigenvalues and eigenvectors. As they have correctly pointed out, their argument is based on translational invariance of the lattice and the $su(2)$ symmetry of the model. Once the $su(2)$ symmetry is broken, e.g. by applying a magnetic field, their argument will not be valid anymore and one may find entanglement in the Heisenberg ferromagnetic chain.

In this paper we show that if we apply a magnetic field to a ferromagnetic Heisenberg chain, then pairwise entanglement will develop between spins at arbitrary given sites. An exact solution of this problem is extremely difficult if not impossible, since as we will see it requires the determination of the spin-spin correlation functions over all the energy eigenstates. However at low temperatures when only the ground state and the first excited states are populated one can calculate the entanglement analytically. Moreover one can now calculate the entanglement profile (entanglement between arbitrary sites) and see its dependence on various control parameters, like the spin coupling, the magnetic field and the temperature. We will find that for finite but arbitrary number of spins, the entanglement profile is a gaussian with a characteristic length depending only on the temperature and the coupling between spins. On the other hand the magnetic field and the total number of spins only affect the amplitude of the profile.

**Remark** Contrary to the case where there is no magnetic field, an exact proof on the presence or absence of entanglement in the Heisenberg ferromagnetic chain is still missing. Exact solutions for up to 4 and numerical evidence for up to 10 spins [1] indicate that there is no entanglement in ferromagnetic chains. If this is indeed the case then the entanglement calculated in this paper should be looked upon not as a result of approximation but as a result of truncation of the spectrum. That is if we somehow prevent the higher excited states from mixing with the low lying states of the Hiesenberg ferromagnet, then we can produce entanglement between different remote sites and suitably manage this entanglement. This problem may be of practical relevance in solid state implementations of quantum computers which should be kept at low temperature to reduce the effect of noise. In such cases we need
to know not only the entanglement between nearest neighbor spins but also between distant spins. The variation of entanglement with distance has not been studied in the works mentioned above, due to the complications in the ground and excited states of the anti-ferromagnetic Heisenberg chain or the Ising model in transverse field. The low lying states of the Heisenberg ferromagnet is a simple situation where we can study this variation.

The structure of this paper is as follows: In section 2 we discuss the general form of the two body density matrix in the Heisenberg chain. In section 3 we review the basic properties of the low lying states of the Heisenberg ferromagnet and in section 4 we calculate the explicit form of the two particle density matrix and its concurrence which characterizes its degree of entanglement. We conclude the paper with a discussion in section 5.

2 Some general properties of the two particle density matrix

The Hamiltonian of the Heisenberg spin chain (1) has the following symmetries

\[ [H, S^z] = [H, \pi] = [H, T] = 0, \]

where

\[ S^z := \frac{1}{2} \sum_{l=0}^{N-1} \sigma^z_l, \]

is the third component of the total spin, and \( T \) is the translation operator

\[ T|s_0, s_1, \cdots s_{N-1}\rangle = |s_1, s_2, \cdots s_{N-1}, s_0\rangle. \]

Here \(|s_i\rangle\), \( s_i = \pm 1 \) is the state of the \( i \)-th spin expressed in terms of the eigenvectors of \( \sigma^z \), i.e. \( \sigma^z_i |s_i\rangle = s_i |s_i\rangle \) and \( \pi \) is the operator which reflects the spin chain around a suitable site: i.e.

\[ \pi|s_0, s_1, \cdots s_{N-1}\rangle = |s_{N-1}, s_{N-2}, \cdots s_0\rangle. \]

This symmetry means that enumerating the sites of the lattice in the clockwise or anticlockwise directions is immaterial for the derivation of the properties of the lattice. The equilibrium state of such a system at temperature \( T \) is given by a density matrix \( \rho = \frac{e^{-\beta H}}{Z} \), where \( \beta = \frac{1}{k_B T} \), \( k_B \) is the Boltzman constant and \( Z = tr(e^{-\beta H}) \) is the partition function.

We are interested in the reduced density matrix and entanglement of two spins at sites \( m \) and \( n \). This is given by

\[ \rho_{m,n} = \frac{1}{Z} tr_{\tilde{m},n} e^{-\beta H}, \]

where \( \tilde{m},n \) means that the trace is taken over all factors in the tensor product space except those at sites \( m \) and \( n \).

From (6) we find various elements of the matrix \( \rho_{m,n} \) as
\begin{equation}
\langle i, j | \rho_{m,n} | k, l \rangle = \frac{1}{Z} \text{tr} \left( e^{-\beta H} (E_{ki}(m)E_{lj}(n)) \right),
\end{equation}

where $i, j, k, l = 0, 1$ and $E_{ki}(m)$ is the operator which acts like $E_{ki} = \langle k | i \rangle$ on site $m$ and like identity on all the other sites. (Note that we use two equivalent notations for the states, namely $|+\rangle = |0\rangle$ and $| - \rangle = |1\rangle$, the $\pm$ notation is usual for the description of spin states and the $|0\rangle, |1\rangle$ notation is usual in description of qubit states in quantum computing.) Expressing the matrices $E_{ki}$ in terms of Pauli matrices and using the symmetry $[H, S^z] = 0$, one can rewrite $\rho_{m,n}$ in terms of correlation functions of spin chains as:

\begin{equation}
\rho_{m,n} = \begin{pmatrix}
n^+ & w & z \\
w & z & w \\
z & w & n^-
\end{pmatrix},
\end{equation}

where due to translational and reflection invariance, the parameters $n^\pm$, $w$ and $z$ depend on $|m - n|$ and

\begin{align*}
n^+ & := \frac{1}{4Z} \text{tr} \left( (1 + \sigma_m^z) (1 + \sigma_n^z) e^{-\beta H} \right) \\
n^- & := \frac{1}{4Z} \text{tr} \left( (1 - \sigma_m^z) (1 - \sigma_n^z) e^{-\beta H} \right) \\
w & := \frac{1}{4Z} \text{tr} \left( (1 - \sigma_m^z) (1 + \sigma_n^z) e^{-\beta H} \right) \\
z & := \frac{1}{2Z} \text{tr} (\sigma_m^\sigma_n^+ e^{-\beta H}).
\end{align*}

For notational convenience we do not show the explicit dependence on $|m - n|$ in the parameters of $\rho_{m,n}$. The equality of the elements $\rho_{01,10}$ and $\rho_{10,01}$, (the reality of $z$) is a consequence of the $\pi$ symmetry and translational symmetry. This is pointed out by Wang and Zanardi in [4], although they explicitly derive this property by the symmetry $[(\sigma^+)^\otimes N, H] = 0$ which exists only in the absence of magnetic field. To see this we temporarily insert the site dependence in the parameters and note that

\begin{align*}
z(m-n) &= \text{tr} (\rho \sigma_m^\sigma_n^+) = \text{tr} (\pi \rho \sigma_m^\sigma_n^+) \\
&= \text{tr} (\rho \sigma_m^\sigma_n^\pi) = \text{tr} (\rho \sigma_{N-m}^\sigma_{N-n}^+) \\
&= \text{tr} (\rho \sigma_{N-n}^\sigma_{N-m}^+) = z^*(N - n - (N - m)) \\
&= z^*(m - n).
\end{align*}

The same argument shows why $\rho_{01,01} = \rho_{10,10}$.

The eigenvalues of this density matrix (which is positive) are $n^\pm$, and $w \pm z$, which implies that the $n^\pm$ and $w$ are positive, while the sign of $z$ is not determined.

The entanglement of the two spins at sites $m$ and $n$ is determined by the concurrence $C(|m - n|)$ defined as

\begin{equation}
C(|m - n|) = \max \{0, \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4\},
\end{equation}

where $\lambda_1, \lambda_2, \lambda_3,$ and $\lambda_4$ are the positive square roots of the eigenvalues of the matrix $\tilde{\rho}_{m,n} \tilde{\rho}_{m,n}$ in decreasing order. The matrix $\tilde{\rho}$ is defined as

\begin{equation}
\tilde{\rho}_{m,n} = (\sigma^y \otimes \sigma^y) \rho_{m,n}^* (\sigma^y \otimes \sigma^y),
\end{equation}

\[ \text{(11)} \]
where \( \ast \) denotes complex conjugation in the computational basis. It turns out that (13)

\[
C(|m - n|) = 2 \max (0, |z| - \sqrt{u^2 + u}).
\]

3 The low lying states of the Heisenberg ferromagnet

The Hamiltonian (1) can be rewritten as

\[
H = JN - 2J \sum_{l=0}^{N-1} P_{l,l+1} + \mu B \sum_{l=0}^{N-1} \sigma_l^z,
\]

where \( P_{l,l+1} \) is the permutation operator acting on sites \( l \) and \( l + 1 \), \( P|s, s'\rangle = |s', s\rangle \).

For the ferromagnetic chain \((J > 0)\), the ground state of \( H \) is the disentangled state

\[
|\epsilon_0\rangle = |-, -, -, \cdot \cdot \cdot, -, -, -\rangle,
\]

where all the spins are down, with energy \( \epsilon_0 = -(J + \mu B)N \).

The first excited states are linear combination of one particle states

\[
|\psi\rangle = \sum_k c_k |k\rangle,
\]

where

\[
|k\rangle := |-, -, -, \cdot \cdot \cdot, +, \cdot \cdot \cdot, -, -, -\rangle,
\]

in which only the spin in the \( k \)-th site is up.

From (11) we find

\[
H|k\rangle = -2J|k - 1\rangle - 2J|k + 1\rangle + (J(4 - N) + \mu B(2 - N))|k\rangle.
\]

leading to the recursion relations for the coefficients

\[
-2J(c_{k-1} + c_{k+1}) + (J(4 - N) + \mu B(2 - N))c_k = \lambda c_k
\]

whose solution together with the periodic boundary condition gives us the final form of the first excited states labeled by \( |\psi_s\rangle \) with \( s = 0 \cdots N - 1 \):

\[
|\psi_s\rangle = \frac{1}{\sqrt{N}} \sum_0^{N-1} e^{\frac{2\pi isk}{N}} |k\rangle,
\]

with energies

\[
\lambda_s = \epsilon_0 + 2\mu B + 8J \sin^2 \frac{\pi s}{N}.
\]

The lowest energy in this band belongs to the flat wave \((s = 0)\) which is higher than the ground state energy by \( 2\mu B \). In the classical picture this is the energy difference due to the flipping of one spin in the magnetic field and there is no contribution from
the interaction of spins. One can guess that the lowest energy in the two particle sector also corresponds to a flat wave, namely to a state

|Ψ⟩ = \frac{1}{\sqrt{\binom{N}{2}}} \sum_{0 \leq i < j \leq N-1} |i,j⟩,

(22)

where |i,j⟩ is a state in which only the spins at sites i and j are up. It is easy to see that this is indeed an eigenstate of the Hamiltonian with an energy \( \epsilon_0 + 4\mu_B \).

Thus if \( \frac{2\mu_B}{kT} \gg 1 \), one may assume that only the ground state and the first excited states will be populated. We will assume that the magnetic field is strong enough and the temperature is low enough so that this condition is fulfilled.

4 Thermal entanglement of two spins

We will calculate the density matrix (6) at low temperatures by taking into account only the ground state and the one-particle eigenstates. At low temperature we approximate various quantities in (9) as follows:

\[
tr(Ae^{-\beta H}) \approx \langle \epsilon_0 | A | \epsilon_0 \rangle e^{-\beta \epsilon_0} + \sum_{s=0}^{N-1} \langle \psi_s | A | \psi_s \rangle e^{-\beta \lambda_s}.
\]

(23)

The operator \( A \) takes one of the following forms, \((1 \pm \sigma_m^z)(1 \pm \sigma_n^z)\), \((1 + \sigma_m^z)(1 - \sigma_n^z)\), or \(\sigma_m \sigma_n^\pm\).

We need the relevant matrix elements over the one particle states. It is easily verified that

\[
\frac{1}{2}(I + \sigma_n^z)|k⟩ = \delta_{n,k}|k⟩,
\]

\[
\frac{1}{2}(I - \sigma_n^z)|k⟩ = (1 - \delta_{n,k})|k⟩,
\]

\[
\sigma_m^+|k⟩ = \delta_{m,k}|k⟩,
\]

(24)

from which we obtain the following matrix elements, where we have used the fact that \( m \neq n \):

\[
\frac{1}{4}\langle \psi_s | (1 + \sigma_m^z)(1 + \sigma_n^z) | \psi_s \rangle = 0,
\]

\[
\frac{1}{4}\langle \psi_s | (1 + \sigma_m^z)(1 - \sigma_n^z) | \psi_s \rangle = \frac{1}{N} \sum_{k,l=0}^{N-1} e^{2\pi i (l-k)s} \delta_{m,k} \delta_{k,l} = \frac{1}{N},
\]

\[
\frac{1}{4}\langle \psi_s | (1 - \sigma_m^z)(1 - \sigma_n^z) | \psi_s \rangle = 1 - \frac{2}{N} e^{\frac{2\pi i (m-n)s}{N}},
\]

\[
\langle \psi_s | \sigma_m \sigma_n^\pm | \psi_s \rangle = \frac{1}{N} e^{\frac{2\pi i (m-n)s}{N}}.
\]

(25)

From \(9\) and \(23\) we find values of different matrix elements of \(\rho_{m,n}\) as follows:
The partition function at this level of approximation is given by

\[ Z \approx e^{-\beta \varepsilon_0} + \sum_{k=0}^{N-1} e^{-\beta \lambda_k} = e^{-\beta \varepsilon_0} + e^{-\beta (\varepsilon_0 + 2\mu B)} \sum_{s=0}^{N-1} e^{-8\beta J \sin^2 \frac{\pi s}{N}}. \]  

(27)

For large \( N \) we can approximate the sums in the above formulas by integrals and at low temperatures (large \( \beta \)) we can evaluate the integrals by saddle point approximation. Thus

\[ \sum_{k=0}^{N-1} e^{-\beta \lambda_k} \approx e^{-\beta (\varepsilon_0 + 2\mu B)} \int_{N/2}^{N} e^{-8\beta J \sin^2 \frac{\pi s}{N}} ds \approx e^{-\beta (\varepsilon_0 + 2\mu B)} N \sqrt{\frac{1}{8\pi \beta J}}. \]  

(28)

The partition function will be

\[ Z \approx e^{-\beta \varepsilon_0} \left( 1 + e^{-2\beta \mu B} N \frac{1}{\sqrt{8\pi \beta J}} \right). \]  

(29)

We also find

\[ \sum_{s=0}^{N-1} e^{2\pi i(m-n)s/N} e^{-\beta \lambda_s} \approx e^{-\beta (\varepsilon_0 + 2\mu B)} \int_{-N/2}^{N/2} e^{-8\beta J \sin^2 \frac{\pi s}{N}} e^{-\frac{2\pi i(m-n)s}{N}} ds \approx e^{-\beta (\varepsilon_0 + 2\mu B)} N \sqrt{\frac{1}{8\pi \beta J}} e^{-\frac{(n-m)^2}{8\beta J}}. \]  

(30)

Putting all this together we find

\[ \rho_{m,n} = \frac{1}{N + \sqrt{8\pi \beta J} e^{2\beta \mu B}} \begin{pmatrix} 0 & e^{-\frac{(n-m)^2}{8\beta J}} \\ e^{-\frac{(n-m)^2}{8\beta J}} & 1 \end{pmatrix} \begin{pmatrix} 0 \ N - 2 + \sqrt{8\pi \beta J} e^{2\beta \mu B} \end{pmatrix}. \]  

(31)
Now that we have the two particle density matrices, we can calculate the entanglement of two spins at an arbitrary distance. From (13) we find

\[ C(|m - n|) = 2|z| = \frac{2}{N + \sqrt{8\pi\beta J e^{2\beta\mu B}}} e^{\frac{(m-n)^2}{4\beta J}}, \tag{32} \]

which can be rewritten as

\[ C(|m - n|) = C_0 e^{-\frac{1}{2} \frac{(m-n)^2}{l^2}}, \tag{33} \]

where

\[ C_0 := \frac{2}{N + \sqrt{8\pi\beta J e^{2\beta\mu B}}} \quad \text{and} \quad l = 2\sqrt{\frac{J}{kT}} \tag{34} \]

denote respectively a scale of the value of entanglement and a kind of entanglement length which determines a scale of length over which the distant spins are still entangled. It is seen that the magnetic field has no effect on the entanglement length and only controls the entanglement amplitude. The higher the magnetic field the lower the value of \( C_0 \). This is understandable since a high value of the magnetic field orders all the spin more in the direction of the \( z \) axis in favor of the disentangled ground state. On the other hand it is the coupling between adjacent spins that entangles distant spins, hence the entanglement length is only affected by \( J \) and \( T \). Raising the temperature has a destructive effect on the entanglement length since thermal fluctuations tend to move the system away from the quantum regime. Finally we note that in the thermodynamic limit when \( N \to \infty \), the concurrence \( C_0 \) tends to zero, so that even the nearest neighbor sites will not be entangled anymore. Figure 1 shows the entanglement profile for a spin chain of \( N = 20 \) spins at two different temperatures.

5  Discussion

As Wang and Zanardi [4] have shown, in the Heisenberg ferromagnet in the absence of a magnetic field there can be no thermal entanglement between nearest neighbor spins. Their argument is based on the \( su(2) \) symmetry of the Hamiltonian. In the presence of a magnetic field this symmetry breaks down to a \( u(1) \) symmetry and one can only derive entanglement by explicitly calculating the relevant thermal correlation functions of the model. We have shown that at low temperatures or high magnetic fields where to a good approximation only the ground state and the one particle states are populated, entanglement can exist between different sites. We have shown that the entanglement profile is a gaussian with an amplitude depending on the magnetic field and temperature and a characteristic length depending only on temperature and the coupling between spins.

Another important point is that in the previous works the pairwise entanglement has been studied in more complicated situations and for making connections to quantum phase transitions, but only for nearest neighbors. By considering the forromagnetic
Figure 1: The concurrence $C$ as a function of $x = |m - n|$, the distance between spins, for a spin chain of $N = 20$ spins at two different temperatures. Solid line ($\mu B / kT = 3, J / kT = 0.6$), dashed line ($\mu B / kT = 4, J / kT = 0.8$).
case and by restricting to the low lying states, we have been able to see how entanglement varies with distance. Knowing this variation may be important for the implementation of quantum protocols on arrays of qubits in any candidate for implementation of quantum computers. An analogous study even for the ground state of the anti-ferromagnetic spin chain is extremely difficult, since it requires the calculation of correlation functions for arbitrary distances and up to now the exact ground state correlation functions of the anti-ferromagnetic model have been calculated for distances of only up to 4 sites [22].

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