Residual Entropy and Low Temperature Pseudo-Transition for One-Dimensional Models

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Here we report an intrinsic relationship between the zero temperature phase boundary residual entropy and pseudo-transition. Usually, the residual entropy increases at the phase boundary, which means the system gains accessible states in the phase boundary compared to its adjacent states, although it is not always the case. Therefore, we propose the following statement at zero temperature. If the residual entropy is continuous at least from the one-sided limit, then the analytical free energy exhibits a pseudo-transition at low temperature. For illustrative purpose, our argument is applied to a frustrated coupled double tetrahedral Ising–Heisenberg chain to show the pseudo-transitions behaviors due to the phase boundary residual entropy continuity.

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1. Introduction

In 1950, van Hove [1] verified the absence of a phase transition for a short-range interaction and uniform one-dimensional system. Using the transfer matrix technique, we can get the free energy, which must be analytic. Therefore, the free energy is analytic. Consequently, the free energy in the thermodynamic limit \( N \to \infty \) becomes

\[
 f = -\frac{1}{\beta} \ln \left( \frac{1}{2} (w_1 + w_{-1}) \right) + \frac{1}{2} \sqrt{(w_1 - w_{-1})^2 + 4w_0^2}. \tag{3}
\]

When \( w_0 = 0 \), Eq. (3) indicates the presence of a genuine finite temperature phase transition at \( w_1 = w_{-1} \).

The organization of this report is as follows. In Sect. 2 the critical residual entropy is presented. In Sect. 3, we study for a double tetrahedral Ising–Heisenberg chain. Finally, in Sect. 4, we present our conclusions.

2. Phase boundary residual entropy

Let us assume that the energies \( \varepsilon_{1,0} \) and \( \varepsilon_{-1,0} \) are the lowest energies for \( n = 1 \) and \( n = -1 \), respectively, and depend on control parameter \( x \), e.g. magnetic field. Thus, the energies \( \varepsilon_{1,0}(x) \) and \( \varepsilon_{-1,0}(x) \), in the critical point become \( \varepsilon_{1,0}(x_c) = \varepsilon_{-1,0}(x_c) = \varepsilon_c \), with its corresponding critical degeneracies at phase boundary as \( g_{1,0} \) and \( g_{-1,0} \). The lowest energy, for \( n = 0 \), satisfies \( \varepsilon_{0,0}(x_c) > \varepsilon_c \), when \( v_0 \to 0 \). Thus, the free energy around the phase boundary becomes

\[
 f = -\frac{1}{\beta} \ln \left( \frac{1}{2} (g_{1,0} + g_{-1,0} + |g_{1,0} - g_{-1,0}|) e^{-\beta \varepsilon_c} \right) = \varepsilon_c - \frac{1}{\beta} \ln \left( \max (g_{1,0}, g_{-1,0}) \right). \tag{4}
\]

Next, we can obtain the corresponding critical residual entropy,
where \( S_c = \ln(\max(g_{1,0}, g_{-1,0})) \),

and from now on, we will consider the entropy in units of \( k_B \). The critical degeneracy per unit cell results in \( G_c = \max(g_{1,0}, g_{-1,0}) \).

It is worth mentioning that, according to the third law of thermodynamics or Nernst’s postulate: The entropy goes to a constant when \( T \to 0 \), and must be independent of any thermodynamic variables such as \( x \).

First, let us assume \( g_{1,0} = g_{-1,0} \), then the residual entropy is \( S(x) = S(x_c) = S_c \). When \( g_{-1,0} < g_{1,0} \), we have \( \lim_{x \to x_c^+} S(x) < \lim_{x \to x_c^-} S(x) = S_c \). Second, we have, \( S_c = \max(g_{1,0}, g_{-1,0}) \), then \( \lim_{x \to x_c^+} S(x) < S(x_c) = S_c \).

In summary, if the residual entropy is continuous at \( x_c \), then the pseudocritical temperature \([5]\) can be determined from the CRE between FR and SA. The CRE between FR and SA is

\[
|\begin{array}{c}
\text{FR1} = \prod_{i=1}^N \left| \begin{array}{c}
\frac{1}{2} - \frac{1}{2} \sigma_i
\end{array} \right|^+, \\
\text{FR2} = \prod_{i=1}^N \left| \begin{array}{c}
\frac{1}{2} + \frac{1}{2} \sigma_i
\end{array} \right|^+
\end{array} \right|
\]

with \( m_I = \frac{1}{2} \), \( m_H = \frac{1}{2} \) and \( m_t = 2 \). (8)

Similarly, the ground state for ferrimagnetic (FI) phase can be expressed as

\[
|\begin{array}{c}
\text{FI} = \prod_{i=1}^N \left| \begin{array}{c}
\frac{1}{2} + \frac{1}{2} \sigma_i
\end{array} \right| -
\end{array} \right|
\]

with \( m_I = -\frac{1}{2} \), \( m_H = \frac{1}{2} \), and \( m_t = 1 \). (9)

The next phase we consider is a frustrated phase, given by

\[
|\begin{array}{c}
\text{SA} = \prod_{i=1}^N \left| \begin{array}{c}
\frac{1}{2} + \frac{1}{2} \sigma_i
\end{array} \right| -
\end{array} \right|
\]

where

\[
\left| \begin{array}{c}
\frac{1}{2} - \frac{1}{2} \sigma_i
\end{array} \right| = \frac{1}{\sqrt{6}} \left( |\uparrow\rangle - 2|\downarrow\rangle + |\uparrow\rangle \right)
\]

or

\[
\left| \begin{array}{c}
\frac{1}{2} - \frac{1}{2} \sigma_i
\end{array} \right| = \frac{1}{\sqrt{2}} \left( |\uparrow\rangle - |\downarrow\rangle \right).
\]

The other frustrated ground state energy is

\[
|\begin{array}{c}
\text{FR2} = \prod_{i=1}^N \left| \begin{array}{c}
\frac{1}{2} + \frac{1}{2} \sigma_i
\end{array} \right|^+
\end{array} \right|
\]

with \( m_I = \frac{1}{2} \), \( m_H = \frac{1}{6} \) and \( m_t = 1 \). (11)

where

\[
\left| \begin{array}{c}
\frac{1}{2} + \frac{1}{2} \sigma_i
\end{array} \right| = \frac{1}{\sqrt{6}} \left( |\downarrow\rangle + 2|\uparrow\rangle - |\uparrow\rangle \right)
\]

or

\[
\left| \begin{array}{c}
\frac{1}{2} + \frac{1}{2} \sigma_i
\end{array} \right| = \frac{1}{\sqrt{2}} \left( |\uparrow\rangle - |\downarrow\rangle \right).
\]

In Fig. 2a, the phase diagram is shown at zero temperature. The CRE between FR1 and FR2 is \( S_c = \ln(3 + \sqrt{5}) \), in units of the Boltzmann constant. In the interface between FR1 and FI we have \( S_c = \ln(3) \). In the same way, the CRE between FI and SA is \( S_c = \ln(2) \), whereas at the boundary between SA and FR2 we have \( S_c = \ln(3) \). All the above critical residual entropies are discontinuous, indicating the absence of the pseudotransition at finite temperature (see Fig. 2b). Finally, the critical residual entropy in the interface of FI and FR2 described by a red solid line is given by \( S_c = \ln(2) \). Therefore, we can affirm that this boundary should lead to a pseudotransition (see Fig. 2b).
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Fig. 2. (a) Zero temperature phase diagram in the plane of \( J_z - h \), assuming fixed parameters \( J = -10 \) and \( J_0 = -10 \). (b) Entropy density plot for temperature \( T = 0.6 \), assuming the same set of parameters considered in (a). Here the prefix letter ‘q’ is to assign the quasi-phases.

Fig. 3. Entropy as a function of \( J_z \) assuming fixed \( J = -10 \), \( J_0 = -10 \), for a range of temperature, \( T = \{0.2, 0.5, 1.0, 1.5, 2.0\} \) (inner to outer curve): (a) for \( h = 20 \), and (b) for \( J_z = -20 \). Density plot of entropy for fixed \( J_z = -10 \): (c) in the plane \( J_z - T \) for \( h = 20 \), and (d) in the plane \( h - T \) for \( J_z = -14.6 \).

To study the thermodynamics of the present model, the Boltzmann factor \( (n = \{-1, 0, 1\}) \) can be expressed as

\[
w_n = 2 \exp \left( \frac{\beta}{4} (2nh - J_z) \right) \times \left[ (e^{\beta J} + 2e^{-\frac{\beta h}{2}}) \cosh \left( \frac{\beta J_0 + h_z}{2} \right) + e^{\beta J_z} \cosh \left( 3\beta J_0 + h_z \right) \right], \tag{12}
\]

In Fig. 3a the entropy is shown as a function of \( J_z \) in the low-temperature region, where we can observe the critical residual entropy between \( FR_2 \) and \( FI \) as \( S_c = \ln(2) \), and this amount remains almost constant up to \( T \lesssim 1 \). This is because the entropy is continuous from the one-sided limit at phase boundary. In Fig. 3b the entropy is plotted as a function of \( h \), where we observe that the residual entropy peaks \( S_c = \ln(4) \) and \( S_c = \ln(2) \) that occur for \( h = 10 \) and \( h = 30 \), respectively. In Fig. 3c we observe well distinct regions up to \( T \lesssim 1 \), and for higher temperature the boundary becomes blurry. Similarly, in Fig. 3d there is a sharp boundary for \( T \approx 0.6 \) and \( 15 \lesssim h \lesssim 25 \). Outside this region thermal excitation destroys any trace of phase transition at zero temperature.

4. Conclusions

Usually, the residual entropy increases in the interface where the phase transition occurs. However, there are some peculiar cases where the critical residual entropy is equal to the largest residual entropy of neighboring states, which is given by \( S_c = \ln(\max(g_{1.0}, g_{-1.0})) \). We can apply this condition at zero temperature, and searching for the continuity of entropy would be an easier task when compared to the study of full thermodynamic quantities. To show this property, we have considered a double tetrahedral Ising–Heisenberg chain.

Acknowledgments

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