Finite size effects around pseudo-transition in one-dimensional models with nearest neighbor interaction

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Abstract

Recently gigantic peaks in thermodynamic response functions have been observed at finite temperature for one-dimensional models with short-range coupling, closely resembling a second-order phase transition. Thus, we will analyze the finite temperature pseudo-transition property observed in some one-dimensional models and its relationship with finite size effect. In particular, we consider two chain models to study the finite size effects; these are the Ising-Heisenberg tetrahedral chain and an Ising-Heisenberg-type ladder model. Although the anomalous peaks of these one-dimensional models have already been studied in the thermodynamic limit, here we will discuss the finite size effects of the chain and why the peaks do not diverge in the thermodynamic limit. So, we discuss the dependence of the finite size effects, for moderately and sufficiently large systems, in which the specific heat and magnetic susceptibility exhibit peculiar rounded towering peaks for a given temperature. This behavior is quite similar to a continuous phase transition, but there is no singularity. For moderately large systems, the peaks narrow and increase in height as the number of unit cells is increased, and the location of peak shifts slightly. Hence, one can naively induce that the sharp peak should lead to a divergence in the thermodynamic limit. However, for a rather large system, the height of a peak goes asymptotically to a finite value. Our result rigorously confirms the dependence of the peak height with the number of unit cells at the pseudo-critical temperature. We also provide an alternative empirical function that satisfactorily fits specific heat and magnetic susceptibility at pseudo-critical temperature. Certainly, our result is crucial to understand the finite size correction behavior in quantum spin models, which in general are only numerically tractable within the framework of the finite size analysis.

1. Introduction

Although one-dimensional models usually do not describe the phase transition at finite temperature, there are some unusual one-dimensional models with a short-range coupling exhibiting a first-order phase transition at finite temperature. Recently, Sarkanych et al.\cite{1} proposed a one-dimensional Potts model with an additional energy degeneracy, which contributes to entropy but not the interaction energy. This extra degeneracy generates a first-order phase transition. The Kittel or zipper model\cite{2}, is a typical simple model whose transfer matrix is finite-dimensional. The zipper model constraint leads to infinite potential, so the free energy becomes a non-analytic function, exhibiting a first-order phase transition. Another model that we can mention is that considered by Chui-Weeks\cite{3}, which was proposed to study the solid-on-solid for the surface growth, whose transfer matrix has an infinite dimension, but still analytically tractable. Imposing the impenetrable condition to subtract, the model shows the existence of the phase transition. The Dauxois-Peyrard\cite{4} is another model with an infinite-dimensional transfer matrix, where some evidence of phase transition has been found. In summary, all those models break the Perron-Frobenius theorem\cite{5} since free energy becomes non-analytical at a critical temperature, or equivalently some elements of the transfer matrix become null (corresponding to an infinite energy).

Previously in the literature, an anomalous property in one-dimensional models with short-range coupling was observed, where an abrupt continuous change comes out in the first derivative of free energy at finite temperature, somewhat similar to the first-order phase transition. Whereas for the second derivative of free energy, an intense giant peak comes into sight, although there is no discontinuity or divergence, which resembles a second-order phase transition. Earlier, in 2011 Timonin\cite{6} called this phenomenon as “pseudo-transition” while studying the spin ice in a field, to indicate a sudden change in the first derivative of free energy, and a vigorous peak in the second derivative of free energy, although there is no discontinuity or divergence, in physical quantities. It is worth noting that the term pseudo-transition is generally used to study finite size lattice systems. Thus, it is possible to observe peaks that increase
with the number of lattice sites, by performing the extrapolation techniques, it is possible to conclude the lattice exhibits a real phase transition in the thermodynamic limit. The results found here are quite similar, for moderately large chain sizes the peak increases proportionally to the chain size, although for chains with a sufficiently large number of unit cells it saturates to a finite value. This fact justifies the name of pseudo-transition.

Lately, this unusual property was discussed in the following recent works. A double-tetrahedral chain of localized Ising spins and mobile electrons show a strong thermal excitation that resembles a first-order phase transition\cite{7, 8}. In the frustrated spin-1/2, Ising-Heisenberg’s three-leg tube exhibited a pseudo-transition\cite{9}. In reference \cite{10}, a similar property was observed when studying thermal entanglement, whose specific heat was reported with a sharp peak on the spin-1/2 Ising-Heisenberg ladder with alternating Ising and Heisenberg inter-leg couplings. This anomalous property was still observed in the spin-1/2 Ising diamond chain in the neighboring of the pseudo-transition\cite{11}. Besides, we also discuss additional properties and further investigations into this peculiar property\cite{12}. As well as that considered distant correlation functions for a spin-1/2 Ising-XYZ diamond chain\cite{13}. An alternative proposal to identify the pseudo-transition was analyzed in the phase boundary residual entropy representation and its finite temperature pseudo-transition relation in one-dimensional models\cite{14}. The universality and pseudo-critical exponents of one-dimensional models were also discussed around the pseudo-transition\cite{15}.

It is valuable to note that the pseudo-transition does not violate the Perron-Frobenius theorem\cite{5}, and guarantees the largest eigenvalues of the transfer matrix are non-degenerate, so free energy becomes an analytical function. Equivalently, some elements (Boltzmann factor) of the transfer matrix become just a tiny amount compared to other elements, or the corresponding energy becomes large enough but finite compared to ground state energy. These types of properties appear more frequently in decorated models\cite{16}. By using somewhat different perspectives, similar anomalous properties have also been discussed in the references\cite{17, 18}.

There is a natural question, how to find a pseudo-critical temperature in quantum spin systems? Such as one-dimensional quantum spin models, quantum spin ladder models\cite{19}, quantum spin tube models\cite{20} or one-dimensional Hubbard models\cite{21, 22, 23, 24}. In this sense, the present work concomitant the proposed technique in reference \cite{14} would useful to elucidate some evidence of pseudo-transition in finite size quantum spin chain. Since most of the quantum spin chain models are only numerically tractable.

We organized this article as follows: In the second section, we present the transfer matrix technique around the pseudo-critical temperature and the finite size effects. In section 3, we discuss Ising-Heisenberg’s tetrahedral chain thermodynamics. In sec 4, we apply for a decorated Ising Heisenberg model in the pseudo-transition vicinity for a finite length chain. We also propose a simple empirical function that fits precisely with exact results. Finally, in section 5, we give our conclusions and perspectives.

2. Transfer matrix

The transfer matrix technique in statistical physics was introduced in 1941 by H. Kramers and G. Wannier\cite{25}. Since then, several lattice models partition functions would be obtained using this technique, where basically, the partition function is written as a sum of all possible micro-states. It also includes an additional summation of each energy level contribution of the system within each micro-state. A somewhat general transfer matrix can always be expressed as a symmetric matrix

\[
V = \begin{bmatrix}
    v_{1,1} & v_{1,2} & \cdots & v_{1,n} \\
    v_{1,2} & v_{2,2} & \cdots & v_{2,n} \\
    \vdots & \vdots & \ddots & \vdots \\
    v_{1,n} & v_{2,n} & \cdots & v_{n,n}
\end{bmatrix},
\]

where the elements are assumed to be \(v_{i,j} > 0\).

Therefore, the partition function becomes

\[
Z_N = \text{tr} \left( \prod_{k=1}^{N} V_k \right) = \text{tr} \left( V^N \right).
\]

In order to obtain the partition function, we must first diagonalize the transfer matrix \(V\), assuming whose eigenvalues are denoted by \(\lambda_r\). So we can express the partition function as follows

\[
Z_N = \sum_{r=1}^{n} \lambda_r^N.
\]
According to the Perron-Frobenius theorem[5, 26], there is a largest non-degenerate eigenvalue $\lambda_1$ of the transfer matrix that satisfy $\lambda_1 > \lambda_r$ with $r = 2, 3, \ldots, n$. Here $N$ stands for the number of sites or unit cells, but it is common in practice to assume $N \to \infty$. However here we focus on exploring the finite size corrections of one-dimensional models.

Using the partition function, we can write free energy per site, as in many textbooks provided by

$$f(N) = -\frac{1}{\beta N} \ln (Z_N) = -\frac{1}{\beta N} \ln \left\{ \lambda_1^N \left[ 1 + \sum_{r=2}^{n} \left( \frac{\lambda_r}{\lambda_1} \right)^N \right] \right\}. \tag{4}$$

Therefore, the free energy(4) can be expressed as follows

$$f(N) = -\frac{1}{\beta} \ln (\lambda_1) - \frac{1}{N\beta} \ln \left[ 1 + \sum_{r=2}^{n} \left( \frac{\lambda_r}{\lambda_1} \right)^N \right], \tag{5}$$

note that each $\frac{\lambda_r}{\lambda_1} < 1$, with $r \geq 2$. Then $\left( \frac{\lambda_r}{\lambda_1} \right)^N \to 0$ when $N \to \infty$, thus the free energy in thermodynamic limit reduces to

$$f = -\frac{1}{\beta} \ln (\lambda_1). \tag{6}$$

In principle, the largest eigenvalue may becomes degenerate $\lambda_1 = \lambda_2$, for some specific control parameters at finite temperature, this would mean the existence of a discontinuous phase transition for a given control parameter. Then undoubtedly, the Perron-Frobenius theorem[5] must be broken. Alternatively, this analysis will be considered in detail below.

2.1. Finite size effects for "quasi-degenerate" largest eigenvalues

Now let us analyze the eigenvalues of transfer matrix using a slightly different perspective. For that purpose, we assume that the Perron-Frobenius theorem[5] is never broken. Therefore, let as back to eq.(5) and assume that $\lambda_2 \to \lambda_1$ (but still $\lambda_2 < \lambda_1$) for some particular control parameter. This means that the largest eigenvalue becomes almost degenerate (quasi-degenerate) but still satisfying the Perron-Frobenius theorem. Taking this fact into account, the free energy provided by (5), can be written as

$$f(N) = f - \frac{1}{N\beta} \ln \left[ 1 + \left( \frac{\lambda_2}{\lambda_1} \right)^N + \sum_{r=3}^{n} \left( \frac{\lambda_r}{\lambda_1} \right)^N \right]. \tag{7}$$

At this limit, the last term within the logarithm of (7) could be properly neglected, for moderately large $N$.

On the other hand, let us denote conveniently a couple of largest eigenvalues by

$$\lambda_{1,2} = e^{-\beta\varepsilon_0} \left( 1 \pm \frac{\zeta}{2} \right), \tag{8}$$

here we assume $\varepsilon_0$ as the lowest energy, and $\zeta$ is a parameter that depends of temperature.

When $\zeta \to 0^+$, we have $\lambda_{1,2} \to e^{-\beta\varepsilon_0}$. This result induces us to believe that there is a degenerate state. Still, according to Perron-Frobenius’s theorem[5], there is no degeneracy, so we name that $\lambda_1$ and $\lambda_2$ are "quasi-degenerate" for a given temperature.

Thereby, we can rewrite the free energy (7) as a function on $\zeta$ and ignoring the last term, we have

$$f(N) = f - \frac{1}{\beta N} \ln \left[ 1 + \left( \frac{1 - \frac{\zeta}{2}}{1 + \frac{\zeta}{2}} \right)^N \right], \tag{9}$$

and here $f$ denotes the free energy in the thermodynamic limit given by (6).

By using the approximate result $\ln(1 - \frac{\zeta}{2}) \approx -\frac{\zeta}{2}$, we can achieve to the following relation,

$$\left( \frac{1 - \frac{\zeta}{2}}{1 + \frac{\zeta}{2}} \right)^N \approx e^{-\zeta N}, \tag{10}$$

where we assume a finite positive $N$.  

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Consequently, the free energy for a finite chain in the vicinity of quasi-degenerate transfer matrix eigenvalues, merely becomes

\[ f^{(N)} \approx f - \frac{T}{N} \ln \left( 1 + e^{-\zeta N} \right). \]  

(11)

This result describes the exact result accurately in the case when the eigenvalues satisfy \( \lambda_2 \to \lambda_1 \) or equivalently \( \zeta \to 0^+ \).

On the other hand, by using the correlation length relation \( \xi = \left[ \ln \left( \frac{\lambda_1}{\lambda_2} \right) \right]^{-1} \), we can express (7) as follows

\[ f^{(N)} = f - \frac{T}{N} \ln \left( 1 + e^{-N/\xi} \right). \]  

(12)

Comparing the free energy (11) and (12), we have the following relation \( \zeta = \xi^{-1} \). However, this result is only valid when \( \zeta \to 0 \).

2.2. Thermodynamic limit close enough to pseudo-critical temperature

For a given temperature, we have \( \zeta \to 0 \) and \( \lambda_1,2 \to e^{-\epsilon_0/T_p} \), which we call pseudo-critical temperature \( T_p \). Therefore, we can express the free energy in thermodynamic limit \( f \) around pseudo-critical temperature, in terms of the variables \( \epsilon_0 \) and \( \zeta \) according to the eqs. (5), thus we have

\[ f = -T \ln(e^{-\beta \epsilon_0}) - T \ln \left( 1 + \frac{\zeta}{2} \right), \]

\[ f = \epsilon_0 - \frac{T \zeta}{2}. \]  

(13)

It is worthy to note that \( \zeta \) depends on the temperature, whose minimum occurs for a given temperature called the pseudo-critical temperature \( T_p \).

Using the free energy provided by (13), we express the entropy

\[ S = -\frac{\partial f}{\partial T} = \frac{\zeta}{2} + \frac{T}{2} \zeta_T, \]

(14)

where \( \zeta_T = \frac{\partial \zeta}{\partial T} \).

Likewise, the specific heat can be obtained as follows

\[ C = -T \frac{\partial^2 f}{\partial T^2} = \frac{T}{2} \left( 2\zeta_T + T\zeta_{T^2} \right), \]

(15)

here we define \( \zeta_{T^2} = \frac{\partial^2 \zeta}{\partial T^2} \).

Since, the magnetization is provided deriving the free energy respect to the magnetic field, which results in

\[ M = -\frac{\partial f}{\partial h} = T \zeta_h, \]

(16)

with \( \zeta_h = \frac{\partial \zeta}{\partial h} \).

Analogously, using the free energy given in (13), we write down the magnetic susceptibility as follows

\[ \chi = -\frac{\partial^2 f}{\partial h^2} = \frac{T \zeta_{h^2}}{2}, \]

(17)

where the second derivative is denoted by \( \zeta_{h^2} = \frac{\partial^2 \zeta}{\partial h^2} \).

This is a crucial point for exploring more cumbersome models, such as quantum Heisenberg spin chain models, in which most of them are only numerically tractable.

2.3. Finite size physical quantities close enough to the pseudo-transition

Our next task is to study the thermodynamics around the pseudo-transition region, taking into account the finite size effects. Below, we can obtain some physical quantities for a finite length chain around the quasi-degenerate or pseudo-transition region, where correlation length can approximately given by \( \xi = \zeta^{-1} \), and using the free energy given by (11), we can obtain the quantities below as a function of \( N \).

The entropy for a finite size chain has the following form,

\[ S^{(N)} = S + \frac{1}{N} \ln \left( 1 + e^{-\zeta N} \right) - \frac{T \zeta_T}{1 + e^{CN}}, \]

(18)
where $S$ means entropy in the thermodynamic limit, while $S^{(N)}$ denotes finite size chain entropy per unit cell. In this region the entropy $S$ describes a strong increase at $T_p$, as we can observe in figs. 2a and 6a, as well as in references\[7, 9, 12, 14, 15\].

Another quantity is the specific heat for a finite size chain, which can be obtained straightforwardly from eq.(18). Hence, around the pseudo-critical temperature it becomes

$$C^{(N)} = C - \frac{T(2\zeta_T + T\zeta_T^2)}{(1 + e^{\zeta_T N})} + \frac{T^2 \zeta_T^2 N e^{\zeta_T N}}{(1 + e^{\zeta_T N})^2},$$

(19)

here $C$ denotes the specific heat in thermodynamic limit given by (15). It is evident that $\zeta > 0$, and when $\zeta \to 0$ means that $\zeta$ has its minimum, so it is reasonable to assume that around the pseudo-critical temperature we must have $\zeta_T \to 0$. Then $C^{(N)}$ reduces to the following expression

$$C^{(N)} = C - \frac{2C}{1 + e^{\zeta_N}} = \left(\frac{e^{\zeta_N} - 1}{1 + e^{\zeta_N}}\right) C = \tanh\left(\frac{\zeta_N}{2}\right) C.$$

(20)

Here, the specific heat $C$ should show a strong sharp peak\[15\] at $T_p$, as illustrated in figs. 2b and 6b.

Next, we express the magnetization for a given a finite size chain

$$M^{(N)} = M - T\zeta_N \left(1 + e^{\zeta_N}\right);$$

(21)

where $M$ is given by (16), which means the magnetization in the thermodynamic limit. Likewise, magnetization must report a strong change at $T_p$.

Straightforwardly, we can also obtain the magnetic susceptibility for a finite size chain,

$$\chi^{(N)} = \chi - \frac{T\zeta_N^2}{(1 + e^{\zeta_N})^2}.$$

(22)

In a similar way to previous case, here we have $\zeta_N = \frac{d\zeta}{dh} \to 0$ in the vicinity of the pseudo-critical transition. And we can surely also ignore the second term, because of $\zeta_N^2 < \zeta_N$.

Therefore, the magnetic susceptibility simply reduces to

$$\chi^{(N)} = \chi - 2\chi - \frac{1 + e^{\zeta_N}}{1 + e^{\zeta_N}},$$

(23)

here $\chi$ is given by (17), which corresponds to magnetic susceptibility in the thermodynamic limit. Simplifying the magnetic susceptibility $\chi^{(N)}$, we achieve to the following simple expression,

$$\chi^{(N)} = \tanh\left(\frac{\zeta_N}{2}\right) \chi.$$

(24)

Magnetic susceptibility might also illustrate a strong acute peak\[15\] close to $T_p$, as illustrated in figs. 2c and 6c.

To check the validity of the results (20) and (24), we will apply for a couple of models in the next sections.

2.4. Finite size correction around $T_p$ for moderately large $N$

For moderately large $N$ and small $\zeta$ (near pseudo-critical temperature), we can still simplify the eq. (20), which becomes

$$C^{(N)} \approx \frac{C}{2} N.$$

(25)

The specific heat (25) indicate that the pseudo-critical peak increases proportionally to $N$, this one resembles the finite size corrections. Consequently, one might naively conclude when $N \to \infty$ leads to divergence, indicating a phase transition. However, it is worth noting that this result fails for considerable large $N$, see eq. (20).

Using similar reasoning, for moderately large $N$ and small $\zeta$, the result given in eq. (24) leads to

$$\chi^{(N)} \approx \frac{\chi}{2} N.$$

(26)

So the magnetic susceptibility increases proportionally to $N$ which again resembles the finite size correction behavior, although, for $N$ sufficiently large, this result also fails accordingly (24).

This analysis may be useful when the system is treated numerically, assuming a finite size chain. It is well known that quantum spin chains are typically investigated using a finite size system. However, here we warn that this analysis must be treated carefully because for $N$ large enough, expressions (25) and (26) fail, so we must use the more general relations (20) and (24), respectively.
3. Ising-Heisenberg tetrahedral chain

Quantum manifestations provided for instance by several real magnetic materials, which can be viewed as one-dimensional systems. Like 3D compounds in which, when we consider one columnar stripe, we could observe a double tetrahedral chain structure. Such as cobalt oxide RbAlCo₄O₇, where R denotes a rare earth atom, which has a swedenborgite lattice structure[27]. Another compound with a similar structure could be the salt with 3D corrugated packing frustrated spin[28] of C₆₀⁻ in (MDABCO⁺)(C₆₀⁻) [MDABCO⁺ = N-methylidiazabicyclooctanum] cation and C₆₀⁻ radical anions, a stripe of this salt can be viewed also as a double-tetrahedral chain.

![Figure 1: Schematic representation of Ising-Heisenberg tetrahedral chain. Small balls (σ_i) corresponds to Ising spins, and large balls (S_a(i), S_b(i)) correspond to Heisenberg spins.](image)

Initially, the Heisenberg tetrahedral chain was studied in reference[29,30]. Later, the Ising-Heisenberg tetrahedral chain (as illustrated in fig[1]), the thermodynamic properties, and for a finite size chain. Thus, the Hamiltonian of the model can be expressed as

\[
H = - \sum_{i=1}^{N} \{ J(S_{a,i}, S_{b,i})z + J(S_{b,i}, S_{c,i})z + J(S_{c,i}, S_{a,i})z + \frac{\hbar}{2} (\sigma_i + \sigma_{i+1}) \}
+ \left( S_{a,i}^z + S_{b,i}^z + S_{c,i}^z \right) \left[ h_z + J_0 (\sigma_i + \sigma_{i+1}) \right],
\]

where \( J(S_{a,i}, S_{b,i})z \equiv J S_{a,i}^x S_{b,i}^x + J S_{a,i}^y S_{b,i}^y + J_z S_{a,i}^z S_{b,i}^z \). With \( S_{a,i}^\alpha \) denoting Heisenberg spin-1/2, and \( \alpha = \{x, y, z\} \), while \( \sigma_i \) denotes the Ising spin \( (\sigma_i = \pm \frac{1}{2}) \). Similarly we define for sites b and c in (27).

3.1. Zero temperature phase transition

Below, we present for didactic reading only a revisit of the zero-temperature phase transition. This model exhibits a peculiar phase transition at zero temperature[14], in which the finite temperature in the vicinity of this phase transition becomes a pseudo-transition. We focus on the peculiar state of zero temperature, the ferrimagnetic (FI) and frustrated (FR) state. Thus, the ferrimagnetic (FI) states can be expressed as

\[
|FI\rangle = \prod_{i=1}^{N} \left( |\uparrow\rangle_i + \frac{1}{\sqrt{2}} |\downarrow\rangle_i \right) |\sigma_i\rangle_i
\]

with Ising spin magnetization \( m_I = -\frac{1}{2} \), Heisenberg spin magnetization \( m_H = \frac{1}{2} \) and total magnetization \( m_T = 1 \). The corresponding energy in the ground state of the ferrimagnetic phase becomes

\[
E_{FI} = \frac{1}{2} (3J_0 + h) - \frac{3L_z}{4} - \frac{3h_z}{2}.
\]

It is certainly worth mentioning that the FI state has zero residual entropy \( (S = 0) \) at zero temperature.

The other state that we are interested in is a frustrated (FR) phase, expressed by

\[
|FR\rangle = \prod_{i=1}^{N} \left( |\frac{1}{2} \rangle_i + \frac{1}{\sqrt{2}} |\frac{1}{2} \rangle_i \right) |\sigma_i\rangle_i,
\]

where

\[
|\frac{1}{2} \rangle_i + \frac{1}{\sqrt{2}} |\frac{1}{2} \rangle_i = \frac{1}{\sqrt{2}} \left( |\uparrow\rangle_i - 2 |\uparrow\rangle_i \right) \text{ or } \frac{1}{\sqrt{2}} \left( |\downarrow\rangle_i - |\downarrow\rangle_i \right),
\]

so the state \( |\frac{1}{2} \rangle_i \) is responsible for the rise of frustration. And the corresponding magnetizations are \( m_I = \frac{1}{2} \), \( m_H = \frac{1}{b} \) and \( m_T = 1 \). Thereby, its respective frustrated ground-state energy becomes

\[
E_{FR} = - \frac{1}{2} (J_0 + h) + \frac{J_z}{2} + \frac{h_z}{2},
\]

Whereas FR state has residual entropy \( S = \ln(2) \) at a zero temperature in units of the Boltzmann constant \( k_B \).
3.2. Thermodynamics of Ising-Heisenberg tetrahedral chain

In order to study the thermodynamic properties of the Hamiltonian \( H \), we can solve this model through the transfer matrix technique. Hence the transfer matrix has the following form \( V = \begin{bmatrix} v_1,1 & v_1,2 \\ v_2,1 & v_2,2 \end{bmatrix} \), whose transfer matrix elements are denoted as \( w_1 = v_1,1 \), \( w_2 = v_2,2 \), and \( w_0 = v_{1,2} \), which are explicitly expressed by

\[
w_n = 2e^{\beta \left( \frac{2h + J_z}{2} \right)} \left\{ \left( e^{3J_z} + 2e^{-\beta J_z} \right) \cosh \left( \beta \frac{nJ_z + J_h}{2} \right) + e^{3J_z} \cosh \left( 3\beta \frac{nJ_z + J_h}{2} \right) \right\}
\]

where \( n = \{-1, 0, 1\} \). With being \( \beta = 1/k_B T \), while \( k_B \) denotes the Boltzmann constant, and \( T \) is the absolute temperature.

Afterward, the eigenvalues of the transfer matrix become

\[
\lambda_{1,2} = \frac{1}{2} \left( w_1 + w_2 \pm \sqrt{(w_1 - w_2)^2 + 4w_0^2} \right).
\]

With this result in our hands, we can express the partition function for the finite size chain as follows

\[
\mathcal{Z}_N = \lambda_1^N + \lambda_2^N.
\]

Using the free energy per unit cell presented in (7) results in

\[
f^{(N)} = -\frac{1}{\beta} \ln(\lambda_1) - \frac{1}{N\beta} \ln \left[ 1 + \left( \frac{\lambda_2}{\lambda_1} \right)^N \right].
\]

Whereas, the free energy in the thermodynamic limit \( (N \to \infty) \) reduces to

\[
f = -\frac{1}{\beta} \ln \left[ \frac{1}{2} \left( w_1 + w_2 + \sqrt{(w_1 - w_2)^2 + 4w_0^2} \right) \right].
\]

This result may indicate the presence of a genuine phase transition at finite temperature when \( w_0 = 0 \), which also means degenerate eigenvalues, since, at this limit, we have \( \lambda_2 = \lambda_1 \).

The phase boundary \( (E_{FI} = E_{FR_2}) \) for \( h_z = h \), restrict the parameters to \( J_z = 2J_0 - J/2 \).

3.3. Finite size effects on pseudo-transition

It is worth mentioning that the residual entropy of the unusual phase boundary at the interface of FI and FR_2 is given by \( S = \ln(2) \). The finite temperature pseudo-transition occurs as a consequence of the zero-temperature phase transition between the ferrimagnetic (FI) and frustrated (FR_2) phase[14].

Here we discuss the pseudo-transition of Ising-Heisenberg tetrahedral chain from a different perspective. For this purpose, we write the free energy in the vicinity of pseudo-critical temperature \( T_p \). As we know from the previous result investigated in reference [12], the pseudo-critical temperature must be obtained using the following relation

\[
w_1(T_p) = w_{-1}(T_p),
\]

where \( T_p \) corresponds to the pseudo-critical temperature. However, it is evident that the condition of \( \lambda_1 > \lambda_2 \) is always satisfied, which guarantees the analyticity of free energy, although pseudo-transition should only occur when \( \lambda_2 \to \lambda_1 \).

In fig. 2a, is illustrated the entropy \( S \) as a function of temperature for a set of values \( N = \{10, 20, 40, 100\} \) and parameters given in the figure legend. Where we observe a continuous step function around pseudo-critical temperature \( T_p \), for small \( N \) the corners of the step function are rounded, as far as \( N \) increases, the rounded corners become increasingly sharp. In fig. 2b, we report the specific heat \( C(T) \) on a logarithmic scale as a function of temperature, for the set of values in panel (a). It is clear how the specific heat peak increases with the number of \( C^{(N)}(T_p) \propto N \) unit cells, and the location of peak shifts slightly, apparently indicating a possible phase transition. The solid black line corresponds to an infinite chain, exhibiting a sharp and robust peak that practically appears to be divergent at a pseudo-critical temperature. The magnetic susceptibility for the Ising spin \( \chi_I = -\frac{\partial^2 f}{\partial h^2} \), and the Heisenberg spin \( \chi_H = -\frac{\partial^2 f}{\partial \lambda^2} \) are almost the same in the neighborhood of the pseudo-critical temperature. So we can just denote by \( \chi(T_p) \equiv \chi_H(T_p) \approx \chi_I(T_p) \). In fig. 2c, the magnetic susceptibility on a logarithmic scale against temperature is reported. In principle, we have a property similar to that illustrated in panel (b).
Figure 2: (a) Entropy as a function of temperature for a set of finite size chains assuming fixed parameters $h = h_z = 20$, $J_0 = -10$, $J = -10$ and $J_z = -14.6$. (b) Specific heat versus $T$, for the same set of parameters in (a). In (c) is depicted the Magnetic susceptibility as function of temperature, for the same set of parameters in (a) and the same set of finite size chain.

Figure 3: (a) $C(T_p)$ and $\chi(T_p)$ as a function of $T_p$ in logarithmic scale. (b) $C(T_p)/\chi_H(T_p)$ and $\chi_I(T_p)/\chi_H(T_p)$ as a function of temperature. In both panels for fixed $h = h_z = 20$, $J_0 = -10$, $J = -10$ and $J_z$ is restricted to $T_p$ by eq. \(37\).

In fig\[3\], the $C(T_p)$ is depicted as a function of $T_p$, which shows how the height of specific heat increases when $T_p$ decreases (blue line). However, when $T_p \to 0$, we have $C(T_p) \to \infty$ then we must have a real phase transition only at $T_p = 0$. Furthermore, magnetic susceptibility $\chi(T_p)$ is illustrated as dependence on $T_p$, which increases monotonically when the pseudo-critical temperature decreases. The peaks are really huge in the low-temperature region (as $T_p \neq 0$), but it is still only a finite peak.

To illustrate an additional property of $C(T_p)$, $\chi(T_p)$ and $\chi_H(T_p)$ we report in fig\[3\] the ratio of $C(T_p)/\chi_H(T_p)$ as a function of $T_p$ represented by a solid blue line, which indicates both quantities are of the same order. Analogously the ratio $\chi_I(T_p)/\chi_H(T_p)$ is depicted by a red line, which reveals almost a constant value around 1; this confirms that both quantities are quite similar around the pseudo-critical peak.

Indeed, this result is valid only in the neighboring of pseudo-critical temperature.

Last but not least, in fig\[4\], we illustrate the specific heat for a finite chain $C^{(N)}(T_p)$ as a function of $N$ in a logarithmic scale, this curve is denoted by circled data obtained from the exact result. The blue line curve describes the function \(20\), which satisfactorily fits with an exact result for all values of $N$. While green line stands for the straight line given by the relation \(25\), and we observe that for $N \lesssim 10^3$ the specific heat increases proportionally to $N$, but for $N \gtrsim 10^3$ fails.

Alternatively, we present a nonlinear empirical function that can also be considered to fit nicely with the exact curve, which is given below

$$C^{(N)}(T_p) \approx \left(1 + \frac{a}{N^b}\right)^{-\frac{1}{4}} C(T_p), \tag{38}$$

where $a \approx 2.829 \times 10^{10}$ is a fitted constant for a fixed $T_p = 0.577077991$. For a moderately large $N \lesssim 10^3$, the empirical expression reduces to $C^{(N)}(T_p) \sim N C(T_p)/\sqrt[4]{a}$, just observing at moderately large $N$, a divergence could be induced when $N \to \infty$, meaning a possible singularity at $T_p$. However, eqs. \(20\) and \(38\) give us the peak dependence for all range of $N$, which at $N \to \infty$, just leads to a finite peak instead of a divergence, this shows that there is no genuine phase transition.
4. Ising-Heisenberg ladder model

Other systems of interest are the spin-1/2 quantum Heisenberg ladder.[33] Some of the most widespread compounds in the spin-1/2 Heisenberg ladder materials literature are cuprates Cu$_2$(C$_8$H$_{12}$N)$_2$Cl$_4$[34], SrCu$_2$O$_2$Cl$_2$[35], (C$_8$H$_{12}$N)$_2$CuBr$_4$[36], and vanadates M$^{2+}$V$_2$O$_5$[37], (VO)$_2$P$_2$O$_7$[38], which involve Cu$^{2+}$ and V$^{4+}$ magnetic ions represented as the spin-1/2 particles. Another compound that is well described by spin-1/2 Heisenberg two-leg ladder is Cu(Qnx)(Cl$_{1-x}$Br$_x$)$_2$, where Qnx stands for quinoxaline (C$_9$H$_8$N$_2$)[39].

As a second application, we consider the model studied in reference[10], although this model has been considered previously, the properties discussed here have not been studied before.

\[ \chi_N(T_p) \approx \left(1 + \frac{a}{N}\right)^{-\frac{1}{2}} \chi(T_p), \]  

with \( a \approx 2.815 \times 10^{10} \) being a fitted constant for a given \( T_p = 0.577077991 \). Again, for moderately large \( N \leq 10^3 \) the eq. (39) reduces to \( \chi_N(T_p) \sim N \chi(T_p)/\sqrt{a} \) which fits nicely, although for \( N \geq 10^3 \) considerably large, it fails.

Figure 5: A schematic representation of the spin-1/2 Ising-Heisenberg ladder model with alternating Ising and Heisenberg inter-leg interactions, thick vertical lines correspond to the Heisenberg coupling (\( J, J_z \)), whereas thin vertical and horizontal lines correspond to the Ising exchange interactions \( J_0 \) and \( J_1 \).

Therefore, let us consider the spin-1/2 Ising-Heisenberg ladder with alternating Ising and Heisenberg inter-leg couplings and the Ising intra-leg coupling schematically depicted in figure 5. The Hamiltonian described above for the spin-1/2 Ising-Heisenberg ladder is given by

\[ \mathcal{H} = - \sum_{i=1}^{N} \left[ J(S_{a,i} S_{b,i})_z + \frac{J_0}{2} (\sigma_{a,i} \sigma_{b,i} + \sigma_{a,i+1} \sigma_{b,i+1}) + \sum_{\gamma = a, b} J_1 (\sigma_{\gamma,i} + \sigma_{\gamma,i+1}) S_{\gamma,i}^z \right], \]

where \( J(S_{a,i} S_{b,i})_z = J(S_{a,i}^z S_{b,i}^z + S_{a,i}^y S_{b,i}^y) + J_z S_{a,i}^z S_{b,i}^z \), with \( S_{a,i}^\alpha \) denotes spatial components of the spin-1/2 operator (\( \alpha = \{x, y, z\} \)) at site i, and \( \gamma = a \) or \( b \) (see figure 5). \( J_1 \) denotes the Ising inter-leg coupling, similarly the Ising intra-leg coupling is denoted by \( J_0 \). Whereas, the anisotropic XXZ Heisenberg inter-leg exchange interaction has two spatial components \( J \) and \( J_z \) in the \( xy \)-plane and along \( z \)-axis, respectively.
4.1. Thermodynamics of Ising-Heisenberg ladder model

To study the thermodynamics of the spin-1/2 Ising-Heisenberg ladder with alternating inter-leg couplings, let us perform the partition function given by [3].

The thermodynamic of the Ising-Heisenberg ladder model can be obtained by the usual transfer matrix approach [25], which has the form,

\[
V = \begin{bmatrix}
v_{1,1} & v_{1,2} & v_{1,2} & v_{1,4} \\
v_{1,2} & v_{2,2} & v_{1,4,u^{-2}} & v_{1,2} \\
v_{1,2} & v_{1,4,u^{-2}} & v_{2,2} & v_{1,2} \\
v_{1,4} & v_{1,2} & v_{1,2} & v_{1,1}
\end{bmatrix},
\]

whose transfer matrix elements are given explicitly by

\[
v_{1,1} = uz (y^4 + y^{-4}) + \frac{u}{z} (x^2 + x^{-2}),
\]

\[
v_{1,2} = z (y^2 + y^{-2}) + z^{-1} (y_1^2 + y_1^{-2}),
\]

\[
v_{1,4} = 2uz + \frac{u}{z} (x^2 + x^{-2}),
\]

\[
v_{2,2} = 2z + \frac{1}{uz} (y_2^2 + y_2^{-2}),
\]

with \(x = e^{\beta J/4}, y = e^{\beta J_1/4}, z = e^{\beta J_2/4}, u = e^{\beta J_3/4}\), and additionally, we define also the following exponential \(y_1 = e^{\beta \sqrt{J^2 + J_0^2}}\) and \(y_2 = e^{\beta \sqrt{J^2 + J_0^2}}/4\).

To find the eigenvalues of the matrix [41], we proceed to calculate the det \((V - \lambda) = 0\). Then, the determinant falls into a secular fourth order equation in \(\lambda\). Factoring this polynomial, we obtain the following expression

\[
0 = (\lambda - v_{2,2} + v_{1,4}u^{-2}) (\lambda - v_{1,1} + v_{1,4}) \times \\
\left[ \lambda^2 - (v_{1,1} + v_{1,4} + v_{2,2} + v_{1,4}u^{-2}) \lambda + (v_{1,1} + v_{1,4}) (v_{2,2} + v_{1,4}u^{-2}) - (2v_{1,2})^2 \right].
\]

After that, the corresponding eigenvalues are expressed as follows

\[
\lambda_1 = \frac{1}{2} \left( w_1 + w_{-1} + \sqrt{(w_1 - w_{-1})^2 + 4w_0^2} \right),
\]

\[
\lambda_2 = \frac{1}{2} \left( w_1 + w_{-1} - \sqrt{(w_1 - w_{-1})^2 + 4w_0^2} \right),
\]

\[
\lambda_3 = v_{2,2} - v_{1,4}u^{-2},
\]

\[
\lambda_4 = v_{1,1} - v_{1,4},
\]

where

\[
w_1 = v_{1,1} + v_{1,4},
\]

\[
w_{-1} = v_{2,2} + v_{1,4}u^{-2},
\]

\[
w_0 = 2v_{1,2}.
\]

In general, as previously assumed, the elements satisfy \(v_{i,j} > 0\). It can be easily seen that the first eigenvalue \(\lambda_1\) is always a positive amount and represents the largest eigenvalue of the transfer matrix. It is obvious to verify that \(\lambda_1 > \lambda_2\), then \(\lambda_1\) is the largest eigenvalue, using the same procedure to that found in ref. [26] [3], it is evident that \(\lambda_3\) is the second largest eigenvalue.

Furthermore, we can write the relations (51-53) explicitly in terms of Hamiltonian parameter

\[
w_1 = 2e^{\beta(J_0 + J_3)} \text{ch} \left( \frac{\beta J_2}{2} \right) + 2e^{\beta(J_0 + J_3)} \text{ch} \left( \frac{\beta J_2}{2} \right),
\]

\[
w_{-1} = 2e^{\beta(J_0 + J_3)} \text{ch} \left( \frac{\beta J_2}{2} \right) + 2e^{\beta(J_0 + J_3)} \text{ch} \left( \frac{\beta J_2}{2} \right),
\]

\[
w_0 = 2e^{\beta J_3} \text{ch} \left( \frac{\beta J_2}{2} \right) + 2e^{\beta J_3} \text{ch} \left( \frac{\beta J_2}{2} \right),
\]
In the thermodynamic limit \( N \to \infty \), the free energy per unit cell \( \frac{F}{N} \) is given only by the largest transfer-matrix eigenvalue, where \( w_1 \), \( w_{-1} \), and \( w_0 \) are given by eqs. (34)–(36). Quantities like entropy or specific heat can be obtained merely from the free energy \( \frac{F}{N} \), by using the standard thermodynamic formulas.

4.2. Finite size effects on pseudo-transition

The Ising ladder model with Ising-Heisenberg intra-rung coupling is characterized indeed by the Hamiltonian \( (10) \), here we explore the phase boundary between two particular phases. These states can be expressed as follows:

The first one is the frustrated phase, which is denoted by

\[
|FRU_i\rangle = \prod_{i=1}^{N} |\tau_i\rangle_i \otimes |\sigma_1^i\rangle_i,
\]

with \( |\tau_i\rangle = \frac{1}{\sqrt{2}} (|+\rangle_i + |-\rangle_i) \) and \( \sigma_1 \) denotes Ising spin orientation, which yields a macroscopically degenerate state. Whereas the corresponding eigenvalue is given by

\[
E_{FRU_i} = -\frac{1}{2}J + \frac{1}{4}J_z - \frac{1}{4}J_0.
\]

The above frustrated phase has a residual entropy \( S = \ln(2) \).

The other state is the antiferromagnetic (AFM) state, which is represented by

\[
|AFM\rangle = \prod_{i=1}^{N} |\eta_i\rangle_i \otimes |+\rangle_i,
\]

with \( |\eta_i\rangle = \frac{(|+\rangle_i + c|\rho\rangle_i)}{\sqrt{1 + c}} \),

and

\[
c = \frac{\sqrt{4J_1^2 + J^2} + 2J_1}{J}.
\]

The corresponding antiferromagnetic eigenvalue results in

\[
E_{AFM} = -\frac{1}{4}J_z - \frac{1}{4}J_1 - \frac{1}{2}\sqrt{4J_1^2 + J^2}.
\]

Obviously, there is no residual entropy for the antiferromagnetic phase.

The phase boundary between \( FRU_1 \) and \( AFM \) has a peculiar interface, since the residual entropy at the border is \( S = \ln(2) \), which becomes the critical residual entropy of the frustrated phase \( S = \ln(2) \), making the residual entropy a continuous function at the phase boundary\[14\]. That is, at this limit, we must observe pseudo-transition at finite temperature.

When the eigenvalues \( \lambda_1 \) and \( \lambda_2 \) becomes almost degenerate \( (\lambda_2 \to \lambda_1) \) in eq. (33), then from the (47) we can get a pseudo-critical condition when \( w_1 - w_{-1} = 0 \), in a similar way to that obtained in eq. (34). Thus, this condition becomes as follows

\[
v_{1,4}(T_p) + v_{1,4}(T_p) = v_{2,2}(T_p) + v_{2,3}(T_p).
\]

In fig \( 6 \), is depicted the entropy as a function of temperature for a finite size chains \( N = \{10, 20, 40, 100\} \) and fixed parameters given in the legend. Here we observe a continuous step function around pseudo-critical temperature \( T_p \), as far as \( N \) increases, the rounded corners of step the function become increasingly acute. In panel (b) is reported the specific heat as a function of temperature for the same set of finite chains and parameters given for (a). Once again, we can observe how the peak increases with the number of sites \( N \), around the pseudo-transition peak. The peak height is clearly sensitive to \( N \), rapidly converging to temperatures higher than the pseudo-critical temperature. Moreover, for \( N \to \infty \), the peak becomes a very sharp peak, quite similar to a continuous phase transition divergence. Whereas in fig \( 6 \), the depict the specific heat as a function of \( N \), which was drawn on logarithmic scale for convenience. The green line illustrates \( C(N) \propto N \left( C(N) = \frac{1}{N} C(N) \right) \), blue line describes the function \( \frac{1}{N} \), while circled curve stands for the exact result. Indeed the specific heat satisfies the finite size correction for \( N \lesssim 10^3 \), while for \( N \gtrsim 10^3 \), the peak height leads to a constant value \( C(T_p) \).
5. Discussion and conclusion

Few one-dimensional models can be solved exactly; in this case, it is natural to study these models already in the thermodynamic limit. But the vast majority of one-dimensional models have no exact solution, so naturally numerical treatments are used to consider the finite size lattice system. Hence, evidence of phase transitions in finite size lattice systems appears as peaks in quantities that depend on the second derivative of thermodynamic potentials. By performing extrapolation techniques, we can identify that the peaks become divergences. Consequently, there is a natural question: what is the relationship between the height of the peak and the finite size chain? Although the one-dimensional models we studied have already been examined in the thermodynamic limit, like decorated models or ladder-type models, the second dimension would manifest itself. In this sense, here we show that the pseudo transitions discussed above have the same origin as finite lattice models in a higher dimension than one, which justifies the name of pseudo-transition. Therefore, we have applied to the Ising-Heisenberg tetrahedral chain and the Ising-Heisenberg ladder model and investigated its finite size effects around pseudo-critical temperature. For sure, both models do not exhibit a genuine phase transition at finite temperature. Despite this, an intense peak emerges in specific heat and magnetic susceptibility at pseudo-critical temperature, closely resembling a second-order phase transition. Still, the system does not exhibit a genuine phase transition at finite temperature. For a moderately large system, the peak depends proportionally on the number of the unit cells. Although, for a sufficiently large system, the height of the peak saturates at a finite value. For most one-dimensional systems, the thermodynamic result is a cumbersome task to get exact solutions. Since, it is common to simulate a finite size system computationally.

The research to find the pseudo-critical temperature in quantum spin chain models is a challenging topic, since, for most one-dimensional models, we cannot get a precise thermodynamic function, which is necessary to observe pseudo-transitions. There is a natural question: observe the pseudo-critical temperature in pure quantum systems? In this sense, our result and together with techniques proposed in reference [1], should be useful to shed light on non-trivial one-dimensional systems such as quantum spin chain models, quantum ladder spin models, quantum triangular tube spin models, one-dimensional Hubbard model[21, 22, 23, 24], or other non-trivial quantum 1d-like systems.

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