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Research note

# High order perturbation study of the frustrated quantum Ising chain

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**Abstract**

In this paper, using high order perturbative series expansion method, the critical exponents of the order parameter and susceptibility in transition from ferromagnetic to disordered phases for 1D quantum Ising model in transverse field, with ferromagnetic nearest neighbor and anti-ferromagnetic next to nearest neighbor interactions, are calculated. It is found that for small value of the frustrating second neighbor coupling ( $k < 0.4$ ), the exponents are the same as those of the classical 2D Ising model ( $\beta = 1/8$ and $\gamma = 7/8$ ), but a deviation from 2D classical Ising universality class is observed for larger values of frustration ( $0.4 < k < 0.5$ ). The reason for this deviation is the "disorder line" which becomes tangent to the Ferromagnetic phase boundary line at $k = 0.5$ .

**Keywords:** quantum phase transition, quantum Ising model, cluster expansion, series expansion, frustrated systems, ANNNI model

## 1. Introduction

The 1D transverse quantum Ising model with ferromagnetic nearest neighbor and anti-ferromagnetic next to nearest neighbor interactions (ANNNI model) is defined by Hamiltonian as:

$$H = -\sum_i \sigma_i^z \sigma_{i+1}^z + k\sum_i \sigma_i^z \sigma_{i+2}^z - \Gamma \sum_i \sigma_i^x \qquad (1)$$

This model is related to the two-dimensional classical ANNNI model through the τ-continuum formalism, hence they belong to the same universality class and a similar phase diagram is expected (if $\Gamma = 0$ is replaced with temperature). The classical axial next-nearest-neighbor Ising (ANNNI) model was introduced by Fisher and Selke [1] to simulate the spatially modulated structures observed in magnetic and ferroelectric systems (for reviews see [2-4]).

The phase diagram of the 1D quantum ANNNI model obtained via analytical and numerical studies is presented in figure 1. It consists of a ferromagnetic phase (FM) phase, a paramagnetic phase (PM) and an antiphase (with a modulated ↑↑↓↓ structure with period 4) and a floating phase (FP) with incommensurate modulation where the spin-spin correlations decay algebraically separating the PM phase from the antiphase. The $k = 0.5$ point on $\Gamma = 0$ axes is a "multiphase point". At the multiphase point the ground state has a very high degeneracy in a sense that any combination of antiphase and ferromagnetic patches will serve as ground-state configuration.

There is also a critical line in the $k < 0.5$ region, given by $\Gamma = k - 1/4k$ , called the "disorder line" [5, 6]. The ground state is exactly solvable on the disorder line, and is given by a direct product of certain spin configurations on each of the sites, i.e., a matrix product state.

Although large parts of the phase diagram of this model are well established, the width and the extension of the floating phase shown in the phase diagram for a quantum ANNNI chain have been a subject of serious debate over last three decades. Generally, there have been three types of conclusions in contrast to each other:
(i) The floating phase, if it exists at all, is restricted to only a line, and extends only over $k > 0.5$ ,
(ii) The floating phase has a finite width, and extends only over $k > 0.5$ ,
(iii) The floating phase extends even for $k < 0.5$ .
To review the papers suggesting the first two conclusions, see [7]. The third conclusion is obtained by Chandra and Dasgupta [8] based on degenerate perturbation calculations in order to investigate the phase that exists near the multiphase point for a nonzero transverse field. They concluded that there exists a floating phase over a region extending from the ferromagnetic phase to the antiphase (for small values of $\Gamma$ ). This result is in contradiction with previous results as none of the previous studies had predicted a floating phase for $k < 0.5$ . In this research, we investigate the universality class of the phase transition

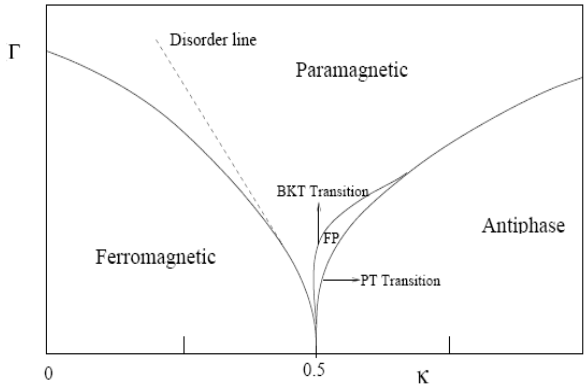


**Figure 1.** Phase diagram of 1D quantum ANNNI model and 2D classical ANNNI model (if $\Gamma$ is replaced with $T$ ), ref. [5].

from ferromagnetic to the paramagnetic phase (or possibly to the floating phase) in $k < 0.5$ region. We perform a high order perturbation expansion (by means of linked cluster expansion method) about the ferromagnetic phase in which the transverse field ( $\Gamma$ ) is considered as perturbation. We obtain the critical line in the phase diagram which separates the ferromagnetic phase from other phases. Across this line, we obtain the critical exponents, $\beta$ for magnetization and $\gamma$ for susceptibility. "Is the universality class of phase transition, i.e. $\beta$ and $\gamma$, the same for all values of $k$ (inside $0 < k < 0.5$ region) or it differs as we vary $k$ ?"

It is found that the critical exponents for $0 < k < 0.4$ belong to the 1D quantum Ising universality class ( $\beta = 1/8$ and $\gamma = 7/8$ ) but a different behavior is observed for $0.4 < k < 0.5$. The reason for this different behavior is explored as well. This result is not informative enough to conclude that phase transition from ferromagnetic phase to floating phase occurs for $0.4 < k < 0.5$. It only states that $0.4 < k < 0.5$ must be treated differently.

## 2. Linked Cluster expansion method and its application to ANNNI model

Cluster expansion method is a general technique for carrying out systematic, high-order perturbation expansions for lattice based quantum many-body systems. At $T = 0$, these expansions require a perturbative diagonalization of infinite dimension matrices. In cluster expansion method the expansion for the infinite system reduces to a sum of terms, each of which involves only a finite cluster and hence a finite dimensional Hilbert space. For a given cluster one constructs the matrices for $H_0$ and $H_1$ in basis in which $H_0$ is diagonal. Expressions for ground state energy and wave function are obtained through elementary recursive relations, and the wave function is then used to evaluate expressions for ground state expectation values. This method is systematic enough to be carried out entirely on the computer [9]. This method is explained in detail in [10, 11].

There are two main steps in a cluster expansion. The first is the identification of the finite number of relevant connected real-space clusters for the Hamiltonian under consideration. Then, for each cluster, one constructs the Rayleigh-Schrodinger perturbation expansion for the extensive quantity (energy, correlation function) under consideration. The results for the various clusters are then combined (via 'subgraph subtraction') so as to yield the quantity per site on the infinite lattice [10].

Suppose that we are interested in calculating an extensive property $P$ for a model defined on a lattice $\mathcal{L}$ . We assume that we are dealing with a large lattice composed of $N$ sites. The key idea in the cluster expansion is to express the quantity $P$, per lattice site, as a sum over all distinct clusters $c$ :

$$\frac{p(\mathcal{L})}{N} = \sum_c L(\mathcal{L}, c) \times W(c) \qquad (2)$$

Here, $L(\mathcal{L}, c)$ is called the lattice constant of the cluster $c$, and is defined as the number of ways per lattice site that the cluster $c$ can be embedded in the lattice. The quantity $W(c)$ is called the weight of the cluster. It is expressed as a power series expansion in the appropriate variable and can be obtained from the relation:

$$W(c) = p(c) - \sum_{g \subset c} L(c, g) \times W(g) \qquad (3)$$

Here $p(c)$ is the series expansion for the property defined on the finite cluster $c$. These equations define the cluster expansion [10].

## 3. Implementation of cluster expansion formalism to the ANNNI Hamiltonian:

In this paper, the first two terms in $H$ are taken to be the unperturbed Hamiltonian ( $H_0$ ) and the third term is taken to be the perturbation Hamiltonian ( $H_1$ ). Cluster expansion formalism expansion about such an unperturbed Hamiltonian is called the "low temperature type expansion", because of the presence of the two-body terms in $H_0$ [9]. If unperturbed Hamiltonian consists of disconnected sites (i.e. there are no two-body terms), expansions about this type of $H_0$ would be "high- temperature type" expansions. In the low temperature perturbation expansions up to order $n$, only clusters with $n$ vertices and less, contribute to the expansion. In a perturbative expansion, generally the $n$-th order correction, the ground state is sum of terms for which, after $n$ iterations, the system gets back to the ground state. Considering the perturbation

$$\sum_i \sigma_i^x = \sum_i \sigma_i^+ + \sigma_i^- \qquad (4)$$

iterations have to make an even number of times on each spin in order to find it in the ground state configuration again. Therefore, the expansions to the ground state properties (which are diagonal in basis of $H_0$ ) will only

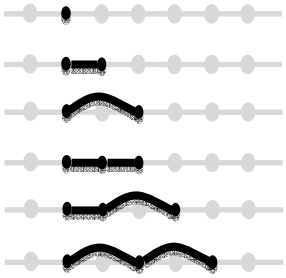

**Figure 2.** All connected clusters up to 3 vertices.

include the even orders. A cluster consisting of $n$ vertices contributes to the order $2n$ and higher. As a conclusion, to obtain the expansion up to $2n$-th order, it would suffice to consider all distinct clusters which have at most n vertices.

As an example, all distinct clusters with the sizes up to 3 vertices are shown in figure 2. Clusters should be considered embedded in the original lattice with ferromagnetic background state. Hence, in computing the unperturbed energy levels, we should include the interactions between the spins within the cluster and also the interactions with spins outside the cluster. The spins outside of the cluster are kept in their unperturbed state, while the perturbation only acts on spins inside the cluster.

In this research we obtain the ground state energy, magnetization and susceptibility up to order 24, which means we generate all distinct clusters which have up to 12 vertices ($2^{12}$ clusters).

## 4. Series analysis and the critical behavior

We use the obtained series to study the critical behavior. For this purpose, standard series analysis methods such as ratio method, padé approximants and integrated differential approximants are developed [12, 13]. Here, we use padé approximation to analyze the series. The goal of this analysis is to extract information from the perturbative series about power-law behavior of the order parameter and the susceptibility close to the critical point in a second order phase transition. Close to the critical point:

$$M = A\left(1-\frac{\Gamma}{\Gamma_c}\right)^{\beta} \quad , \tag{5}$$

$$\chi = \frac{B}{\left(1-\frac{\Gamma}{\Gamma_c}\right)^{\gamma}} \quad .$$

For example, consider a perturbative expansion for the order parameter

$$M = a_0 + a_1\Gamma + \ldots + a_N\Gamma^N \sim A\left(1-\frac{\Gamma}{\Gamma_c}\right)^{\beta} \tag{6}$$

$$\frac{d}{d\Gamma}\log M = b_0 + b_1\Gamma + \ldots + b_{N-1}\Gamma^{N-1} \sim \frac{\beta}{\Gamma_c - \Gamma}$$

The goal of padé approximation is to use the coefficients

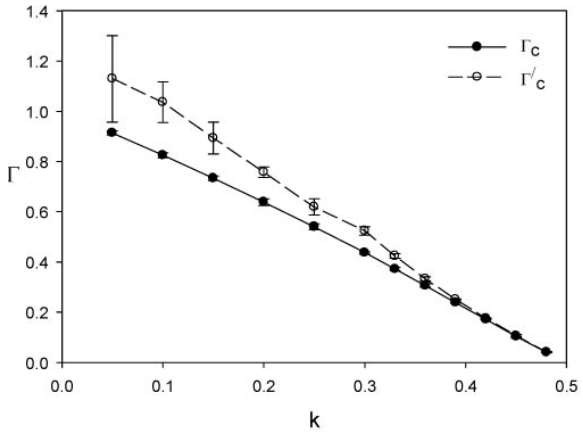


**Figure 3.** Critical points of magnetization ( $\Gamma_c$ and $\Gamma_c^{'}$ ) versus $k$.

$a_0,\ldots,a_{N-1}$ or $b_0,\ldots,b_{N-1}$ to estimate $\Gamma_c$, $\beta$ and $A$. This is done by converting series to a rational expression of two polynomials:

$$b_0 + \ldots + b_{N-1}\Gamma^{N-1} \sim \frac{c_0 + \ldots + c_L\Gamma^L}{1 + d_1\Gamma + \ldots + d_M\Gamma^M} = \frac{P_L}{Q_M} \tag{7}$$

This has a unique solution for all $c_j$ and $d_j$ coefficients if $L + M \le N - 1$ and all we have to do is to solve a set of linear equations. The critical point $\Gamma_c$ is considered to be one of roots of the dominator polynomial $Q_M$. There are ways to distinguish the actual critical point $\Gamma_c$ from the other nonphysical roots of $Q_M$. For example, the nonphysical roots of $Q_M$ either happen in the nonphysical range of $\Gamma$ or coincide with zeroes of $P_L$. Also the actual critical point appears frequently when we apply different padé approximations i.e. when we vary $L$ and $M$. Such critical points sometimes are called poles of the series. After $\Gamma_c$ is approximated the critical exponent $\beta$ and the amplitude $A$ can be estimated by simple extrapolations.

Another point about the series analysis is that there is often more than one pole (critical point) appearing in various padé approximants. Appearing many poles usually weakens the analysis and increases the errors, especially if there are two poles close to each other. This is the case for our analysis. As we will see later, in both Magnetization and susceptibility series, there are two poles close to each other. In such conditions, the best approximations are made for the pole which is the closest to the origin ( $\Gamma = 0$ ). The second pole is not physical i.e. it cannot be associated with an actual physical phase transition but it is important because it influences the behavior of the actual critical point in which the physical phase transition occurs.

In the next pages, we present the results of analysis for magnetization and susceptibility series.

## 5. Critical behavior of magnetization

We use the following relation to obtain the critical exponent of magnetization:

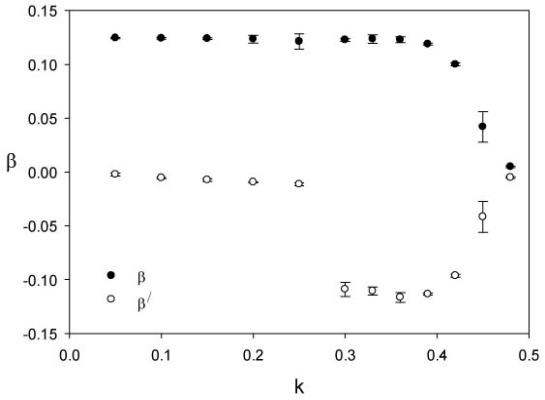


**Figure 4.** $\beta$ and $\beta^{'}$ versus $k$.

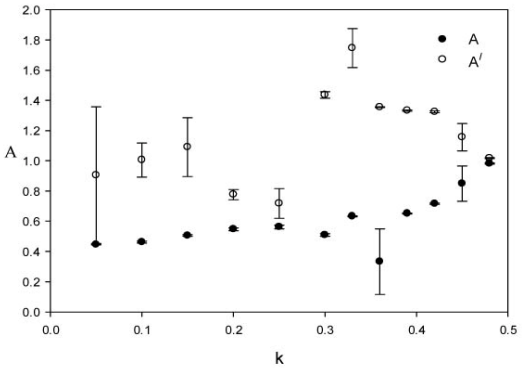


**Figure 5.** $A$ and $A^{'}$ versus $k$.

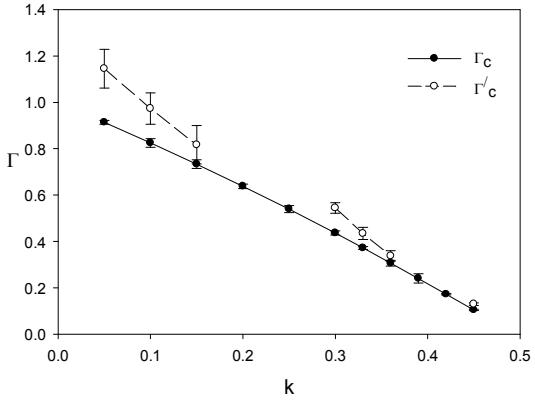


**Figure 6.** Critical points of susceptibility ($\Gamma_c$ and $\Gamma_c^{'}$) versus $k$.

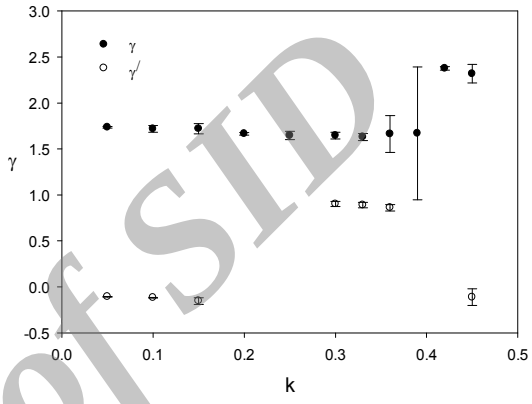


**Figure 7.** $\gamma$ and $\gamma^{'}$ versus $k$.

$$M \sim A\left(1-\frac{\Gamma}{\Gamma_c}\right)^{\beta}+A^{'}\left(1-\frac{\Gamma}{\Gamma_c^{'}}\right)^{\beta^{'}} \qquad (8)$$

The calculated values of $\Gamma_c$ and $\Gamma_c^{'}$ ($\Gamma_c^{'} \geq \Gamma_c$) are presented in figure 3. Also, the relative critical exponents ($\beta$ and $\beta^{'}$) and amplitudes ($A$ and $A^{'}$) are presented in figures 4 and 5.

The observed critical behavior can be summarized in three steps:

(i) $0 < k < 0.3$

There is a critical point at $\Gamma_c$ with critical exponent $\beta = 1/8$, which is the standard critical exponent of the order parameter for 1D quantum Ising (or 2D classical Ising) universality class. There is also a second weak singularity at $\Gamma_c^{'}$ with $\beta^{'} \approx 0$ which gets closer to the first singularity as k increases but it doesn't influence the nature of the main singularity. We should note that $\beta^{'} \approx 0$ could mean logarithmic correction to the power law scaling behavior, i.e. $A^{'}\log\left(1-\Gamma/\Gamma_c^{'}\right)$.

At some point in range $0.25 < k < 0.30$ the nature of the second singularity undergoes a sudden change and there is a considerable jump in $A^{'}$ and $\beta^{'}$ at $k = 0.3$ point. As we will see in the conclusions part, this is because beyond $k > 0.3$ the well-known "disorder line" crosses the weak singularity line and gets closer to the ferromagnetic phase boundary line.

(ii) $0.3 < k < 0.4$

In this range $\beta = -\beta^{'} = 1/8$ and magnetization can be expressed by

$$M \sim \left(\frac{\Gamma_c-\Gamma}{\Gamma_c^{'}-\Gamma}\right)^{1/8},$$

(iii) $0.4 < k < 0.5$

In this range

$$M \sim \left(\frac{\Gamma_c-\Gamma}{\Gamma_c^{'}-\Gamma}\right)^{\beta}.$$

As we get closer to the $k = 0.5$ point,

$\Gamma_c^{'} \to \Gamma_c$ ,

$\beta \to 0$ ,

$A, A^{'} \to 1$ .

The second singularity (the disorder line) in the phase diagram becomes tangent to the main singularity. This influences the critical exponent of the actual phase transition. As you can see (figure 4), $\beta$ gradually vanishes as we get closer to $k = 0.5$ and it differs from the 1D quantum Ising universality class.

## 6. Critical behavior of susceptibility

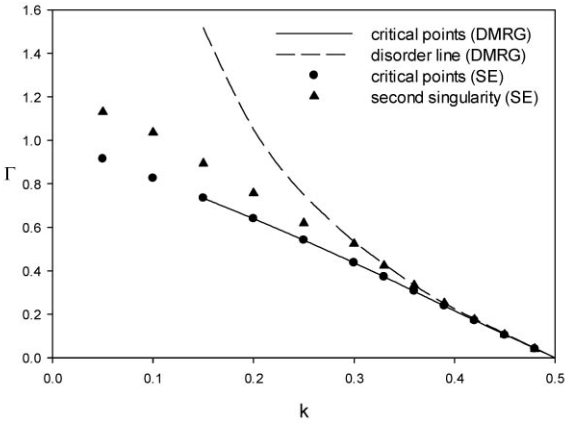


**Figure 8.** The phase diagram obtained by SE (this research) and DMRG [6]

of susceptibility using a symbolic function

$$\chi \sim \frac{B(\Gamma)}{\left(1-\frac{\Gamma}{\Gamma_c}\right)^{\gamma}\left(1-\frac{\Gamma}{\Gamma_c^{'}}\right)^{\gamma^{'}}} \quad , \tag{9}$$

In which $\Gamma_c$ , $\Gamma_c^{'}$ and $\gamma$ , $\gamma^{'}$ are presented in figures 6 and 7. Just like magnetization, there are two singularities. The main singularity is associated with the critical exponent $\gamma \approx 1.75$ for $k < 0.4$. This is the standard critical exponent expected for the 1D quantum Ising universality class. For $k > 0.4$ , there seems to be a jump in the critical exponent. One can see how this jump is influenced by the second singularity (the disorder line).As we get closer to the $k = 0.5$ point, the second singularity with $\gamma^{'} \approx 0.85$ gets closer to the main singularity. Beyond $k > 0.4$ the two singular point get so

Just like magnetization, we express the critical behavior close that

$$\lim_{\Gamma_c^{'} \to \Gamma_c} \left(1-\frac{\Gamma}{\Gamma_c}\right)^{\gamma}\left(1-\frac{\Gamma}{\Gamma_c^{'}}\right)^{\gamma^{'}} = \left(1-\frac{\Gamma}{\Gamma_c}\right)^{\gamma+\gamma^{'}}$$

This explains the jump in the critical exponent.

## 7. Conclusions

It is found that the critical exponents for $0 < k < 0.4$ belong to the 1D quantum Ising universality class ( $\beta = 1/8$ , $\gamma = 7/4$ ) but a different behavior is observed for $0.4 < k < 0.5$ . The reason for this different behavior is explored as well: the disorder line becomes tangent to the FM phase boundary line as we get closer to $k = 0.5$ . This changes the nature of phase transition, i.e. the critical exponents differ from the expected values.

We present the phase diagram obtained by this research accompanied by the result of a DMRG study [6] in figure 8. As you can see, the FM phase boundary line obtained from series expansion (SE) and DMRG are identical. Series expansion detects another weak singularity for $k < 0.3$ which gives its place to the disorder line beyond $k > 0.3$ . The agreement between the two methods (and theory) on the disorder line (beyond $k > 0.3$ for SE) is remarkable.

Nature of the second singularity (triangles in $k > 0.3$ region) remains unresolved. Unfortunately, this can not be studied using series expansion method anymore, but we suggest finite size studies around triangles. This line could be the boundary between two different paramagnetic phases or the boundary of the floating phase and paramagnetic phase as ref. [8] suggests.

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