Phase diagram of the anti-ferromagnetic xxz model in the presence of an external magnetic field

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Abstract

The anisotropic $s = \frac{1}{2}$ anti-ferromagnetic Heisenberg chain in the presence of an external magnetic field is studied by using the standard quantum renormalization group. We obtain the critical line of the transition from partially magnetized (PM) phase to the saturated ferromagnetic (SFM) phase. The crossover exponent between the PM phase and anti-ferromagnetic Ising (AFI) phase is evaluated. Our results show that the anisotropy($\Delta$) term is relevant and causes crossover. These results indicate that the standard RG approach yields fairly good values for the critical points and their exponents. The magnetization curve, correlation functions and the ground state energy per site are obtained and compared with the known exact results.

PACS numbers: 05.50.+q,75.10.-b,75.10.Jm
Keywords: Quantum renormalization group, Spin systems, Heisenberg model.

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1 Introduction

Systems near criticality are usually characterized by fluctuations over many length scales. At the critical point itself, fluctuations exist over all scales. At moderate temperatures quantum fluctuations are usually suppressed compared with the thermal fluctuations. However if the temperature is near zero, the quantum fluctuations especially in the low-lying states dominate the thermal ones and strongly influence the critical behaviour of the systems. The study of the ground state and its energy is thus of central importance for understanding the critical behaviour of such systems.

The technique of Renormalization Group (RG) has been so devised to deal with these multi-scale problems\cite{1, 2, 3, 4}. In the momentum space RG which is suitable for studying continuous systems one iteratively integrates out the small scale fluctuations and renormalizes the Hamiltonian. In the real space RG, which is usually performed on lattice systems with discrete variables (i.e. quantum spin chains), one divides the lattice into blocks which are treated as the sites of the new lattice\cite{5}. The Hamiltonian is divided into intra-block and inter-block parts, the latter being exactly diagonalized, and a number of low lying energy eigenstates are kept to project the full Hamiltonian onto the new lattice. The accuracy of the method is determined by the number of states kept and specially is sensitive to the boundary conditions\cite{4, 6, 7} which is considered for the block Hamiltonian. The detailed form of this projection in fact differentiates various versions of the real space RG, ranging from the standard RG to the recent Density Matrix RG (DMRG)\cite{9}. Each of these versions have their own advantage and disadvantages.

The Ising model in a transverse field (ITF) and anisotropic XY model in a transverse field (AXYTF) have been studied in \cite{10, 11} using both standard RG and DMRG methods. There, it has been concluded that DMRG gives accurate results for the ground state energy and correlation functions in both models, but the standard RG method where the number of states kept are not few can give better results in determining the location of critical points and critical exponents. In this direction we have been motivated to study a more general model, the anisotropic Heisenberg model in the presence of an external magnetic field ($xxz+h$) by using the standard RG method to compare its results with the known
exact ones. This RG study allows us to have analytic RG equations which gives a better understanding of the behaviour of the real space RG method at the critical points. We have studied the $xxz+h$ model because of its richness in the phase-diagram where there are different critical behaviour. In this study we have succeeded to obtain the critical line between the partially magnetized (PM) and saturated ferromagnetic (SFM) phases, to a good accuracy, compared with the known results\cite{12}. We have also derived the crossover between the PM phase (small anisotropy $-1 < \Delta < 1$) and the anti-ferromagnetic Ising (AFI) phase (large anisotropy $\Delta >> 1$) and calculated its exponent ($\phi > 0$) which verifies the relevance of anisotropy to the crossover phenomena. These results which come out of an RSRG by keeping only two states in each block confirm that RSRG is a good candidate to study at least the qualitative behaviour of the quantum lattice systems in the quantum critical region.

In this letter we have studied the $xxz+h$ model by RSRG method where the block length is three ($n_B = 3$). In the next section we will introduce the $xxz+h$ model and discuss its critical behaviour as derived by other methods. In section 3 we will discuss about different types of constructing RG–equations and obtain the analytic RG–equations for this model. Using these equations we will describe the phase-diagram of this model. We will discuss the critical behaviour of the $xxz+h$ model by RG–equations in section 4. In section 5 we will compare some of the results i.e. ground state energy and correlation functions with the known exact results. The paper ends with a conclusion.

2 The Model

The anisotropic spin $\frac{1}{2}$ anti-ferromagnetic Heisenberg model, or $xxz$ chain is one of the most studied quantum spin systems in statistical mechanics. It is also a classic example of one dimensional integrable quantum spin systems\cite{12, 13, 14}. The $xxz$ chain gives us the first example of a critical line with critical exponents varying continuously with the anisotropy. The model has also been studied by using the conformal invariance idea\cite{15}, where the critical fluctuations along the critical line are governed by a conformal field theory with central charge $c=1$. The RG study of $xxz$ model has been performed by Rabin\cite{16}. At
Δ = 0, even in the presence of magnetic field, the model can be mapped by Jordan–Wigner transformation to free–fermions[17], which is exactly solvable. This system has also been studied within the RG formalism[11].

The Hamiltonian in the presence of an external magnetic field is

\[
H(J, \Delta, h) = J \sum_{i=1}^{N} (s^x_i s^x_{i+1} + s^y_i s^y_{i+1} + \Delta s^z_i s^z_{i+1} + hs^z_i)
\]  (1)

where \( J > 0 \), \( \Delta \) is the anisotropy parameter, which in the anti-ferromagnetic region is taken to be greater than or equal to \(-1\), and \( h > 0 \) is the strength of the external magnetic field. The effect of a uniform magnetic field in the phase diagram of the \textit{xxz} chain is to extend the critical phase over a finite region which is partially magnetized and delimited by a critical line where the chain becomes saturated ferromagnetic[12, 15]. Uniform external magnetic field does not destroy the exact integrability of the quantum chain but the coupled integral equations for the spectral parameter do not have closed analytic solutions. Then the only results are numerical or perturbative ones[12, 14, 15].

The Hamiltonian \( H(J, \Delta, h) \) is related by a canonical transformation \( U = e^{i\pi \sum_{j=1}^{N} js^z_j} \) to \( H(J, -\Delta, h) \), i.e. \( UH(J, \Delta, h)U^{-1} = -H(J, -\Delta, h) \). This gives a relation between the antiferromagnetic(\( J > 0 \)) and ferromagnetic(\( J < 0 \)) cases. At \( \Delta = 1 \) and \( h = 0 \) the Hamiltonian exhibits an su(2) symmetry. For \( \Delta \neq 1 \), it exhibits a quantum symmetry \( su_q(2) \)[18]. If \( h \neq 0 \), the only symmetry is U(1). Let us now begin the RG study of the \textit{xxz+h} model.

3 Renormalization Group Equations

The implementation of RSRG is based on two important points, the size of blocks and the number of states kept in each step of RG. Both of them would have significant effects on the RG flow. Here we choose a 3-sites block(\( n_B = 3 \)) for the renormalization process. In this case the two lowest energy states of the block Hamiltonian preserve the symmetries of the Hamiltonian and lead to a self similar Hamiltonian. Moreover at large \( \Delta \) and \( h \) the level crossing of the ground state in the block occurs at a coupling constant which is exactly its critical value (this will be explained latter, see also appendix). Finally taking larger blocks, renders an analytic RG–equations, difficult to obtain.
After dividing the whole chain into 3-sites blocks, the first step of RSRG is to divide the Hamiltonian into two parts, the intra–block Hamiltonian \((H^B)\) and the inter–block Hamiltonian \((H^{BB})\). There are several choices for doing this decomposition. In our prescription we choose the decomposition which is sketched in fig.1. In this case the block Hamiltonian is

\[
H^B_\mu = J[s_1^x s_2^x + s_2^x s_3^x + s_1^y s_2^y + s_2^y s_3^y + \Delta(s_1^z s_2^z + s_2^z s_3^z) + h(s_1^z + s_2^z + s_3^z)],
\]

where \(\mu\) represents the block number i.e. \(H^B = \sum_{\mu=1}^{N/3} H^B_\mu\). The block Hamiltonian is diagonalized exactly and then the two lowest lying states are kept to span the truncated (or effective) Hilbert space. Thus the embedding operator \(T\) is constructed to be

\[
T = |\alpha\rangle \langle + | + |\beta\rangle \langle - |
\]

where \(|\alpha\rangle\) and \(|\beta\rangle\) represent the two low-lying eigenstates of \(H^B\) and \(|+\rangle, |\rangle\) are the renamed base kets for the effective Hilbert space.

There is a level crossing at \(h = h_0\) (eq.(5)) in the spectrum of \(H^B_\mu\), where the ground state changes from the \(S^z = -\frac{1}{2}\) state to the \(S^z = -\frac{3}{2}\) state \((S^z = s_1^z + s_2^z + s_3^z)\). Note that \(h_0\) comes from the finite size effects of a 3-sites block and reaches the critical value of external magnetic field \((h_c)\) by increasing the block sizes \((n_B \to \infty)\). In that case the ground state changes from a PM state \((m \neq 0)\) to a SFM state \((|m| = 0.5)\). Thus in the absence of magnetic field, the ground state of the block Hamiltonian is a spin \(\frac{1}{2}\) doublet. As \(h\) is turned on weakly, we enter in a Zeeman regime and the doublet splits into two states. This is true as long as \(h < h_0\). For strong magnetic fields, we are in a regime in which the ground state is a singlet with all spins down. This should correspond to \(h > h_0\). The results of this computation are as follows : for \(h < h_0\):

\[
|\alpha\rangle = b|++\rangle + a|--\rangle + b|\rangle - ++),
\]

\[
|\beta\rangle = -b|--\rangle - a|\rangle - ++) - b|++\rangle,
\]

where

\[
h_0(\Delta) = \frac{3\Delta + \sqrt{\Delta^2 + 8}}{4},
\]
\[ a = \frac{2x + 2}{\sqrt{6 + 12x^2}} \quad , \quad b = \frac{2x - 1}{\sqrt{6 + 12x^2}} \]

and

\[ x = \frac{2(\Delta - 1)}{8 + \Delta + 3\sqrt{\Delta^2 + 8}} \]

for \( h > h_0 \):

\[
|\alpha\rangle = -b|---\rangle - a|--+\rangle - b|+-+\rangle, \quad (6)
\]

\[
|\beta\rangle = |---\rangle . \quad (7)
\]

Having the embedding operator at hand, the operators (observables) are renormalized as

\[ O' = T^\dagger OT. \quad (7) \]

By using the above equation one can obtain the renormalization of operators. Thus for \( h < h_0 \) we obtain the following relations : \((h < h_0)\)

\[
T^\dagger s^x_{1(3)} T = -2abs^{sx} \quad ; \quad T^\dagger s^x_{2} T = -2b^2 s^{tx}
\]

\[
T^\dagger s^y_{1(3)} T = 2abs^{sy} \quad ; \quad T^\dagger s^y_{2} T = 2b^2 s^{ty}
\]

\[
T^\dagger s^z_{1(3)} T = a^2 s^{sz} \quad ; \quad T^\dagger s^z_{2} T = (1 - 2a^2) s^{tz}
\]

We find the same renormalization for \( s_1 \) and \( s_3 \) because of the symmetry in site 1 and 3 in the block \((1—2—3)\). We will obtain similar relations for \( h > h_0 \):

\[
T^\dagger s^x_{1(3)} T = -bs^{sx} \quad ; \quad T^\dagger s^x_{2} T = -as^{sx}
\]

\[
T^\dagger s^y_{1(3)} T = bs^{sy} \quad ; \quad T^\dagger s^y_{2} T = as^{sy}
\]

\[
T^\dagger s^z_{1(3)} T = -\frac{a^2 + 1}{4} I + \frac{1 - a^2}{2} s^{sz} \quad ; \quad T^\dagger s^z_{2} T = \frac{a^2 - 1}{2} I + a^2 s^{tz}.
\]

In the above equations \( s^{\alpha} \) is the effective operator in the effective Hilbert space of the block (new sites in the renormalized chain). By considering the interaction between blocks and using the above equations \((8),(9)\) we will obtain the renormalization of coupling constants in the Hamiltonian:

\[
|h| < h_0(\Delta) : \quad \begin{cases} 
J' = 4a^2b^2 J, \\
\Delta' = \frac{a^2}{4a^2} \Delta, \\
h' = \frac{1}{4a^2b^2} h, 
\end{cases} \quad (10)
\]
The above RG–equations show that the renormalized Hamiltonian is of the same form as the original one. The critical behaviour which can be obtained from these equations will be discussed in the next section.

Let us consider an extreme case where both \( h \) and \( \Delta \) go to infinity and \( J \) goes to zero such that \( J\Delta, Jh \) and \( \frac{h}{\Delta} \) remain finite. In this case the Hamiltonian reduces to a simple anti-ferromagnetic Ising (AFI) model in the presence of an external magnetic field, which shows a first order transition from a classical anti-ferromagnetic (Neel) ordered phase \( (m = 0, sm = \frac{1}{N} \sum_i (-1)^i s_i^z = 0.5) \) to a saturated ferromagnetic phase (SFM) \( (|m| = 0.5, sm = 0) \).

We can write this Hamiltonian as

\[
H_{AFI} = k \sum_i (s_i^z s_{i+1}^z + g s_i^z)
\]

where

\[
k = J\Delta > 0 \quad , \quad g = \frac{h}{\Delta}
\]

At large \( \Delta (\Delta >> 1) \) we have \( h_0 \simeq \Delta \), \( a \to 1 \) and \( b \to 0 \). Then the RG–equations reduces to the following equations.

\[
|h| < \Delta : \quad \begin{cases} J' = 4b^2 J, \\ \Delta' = \frac{1}{4b^2} \Delta, \\ h' = \frac{1}{4b^2} h, \end{cases}
\]

\[
|h| > \Delta : \quad \begin{cases} J' = b^2 J, \\ \Delta' = b^2 \Delta, \\ h' = \frac{1}{b^2} (|h| - \Delta) \text{sgn}(h). \end{cases}
\]

These RG–equations give exactly the critical point \( g_c = 1 \) and the ground state energy of the AFI model(see appendix), which will be discussed in the next section.
4 Critical Behaviour

In this section we analyze the RG–equations and its critical behaviour. The phase diagram of
the obtained RG–flow(eqs.(10,11)) is depicted in fig.2. This phase diagram consists of three
different phases, partially magnetized (PM), classical anti-ferromagnetic(AFI) and saturated
ferromagnetic (SFM) phases.

There are five fixed points in the phase diagram,

(i) XX represents a spin $\frac{1}{2}$ xx model without external field,

(ii) XXTF is the critical point of the xx model in the presence of a transverse field,

(iii) IAFH represents the critical point of the xxz model in the absence of an external field,

(iv) AFI represents a classical anti-ferromagnetic Ising model with a long-range Neel order,

(v) SFM represents a saturated ferromagnetic phase where all spins align in the direction of
the external field.

In the SFM phase the RG–flow has a well defined behaviour and goes to the SFM fixed
point for any value of $h > h_c(\Delta)$. But when $h < h_c(\Delta)$ and $-1 \leq \Delta \leq 1$ the RG–flow
represent a massless phase in which $J^{(n)} \to 0$ and $\Delta^{(n)} \to 0$ in the limit $n \to \infty$ ($n$ is the
number of RG steps). The RG flow in the PM phase has a cyclic nature. Since it reflects
a sequence of level crossings between states with different values of the total $S^z$ induced by
varying the magnetic field. The recurrence of this level crossing in the process of RG leads
to the oscillatory behaviour of the RG flow. If we imagine of a 3–dimensional RG flow, its
projection onto the $h−\Delta$ plane will have some closed paths. However if the initial point is
in the PM(or SFM) phase, it will go to the XX(or SFM) fixed point finally. Therefore we
conclude that the RG flow in the PM phase can be sketched as in fig.2. At the end of this
region on the $\Delta = 0$ line there exists a fixed point at $h_c = 0.943$ which separates the PM and
SFM phases. The eigenvalues of RG–flow at this critical point are given in table-1, which
give a relevant direction on the $\Delta = 0$ line and an irrelevant direction along the critical line
$h_c = 0.943\Delta + 0.943$. This critical line is obtained from the behaviour of the correlation
functions. We have calculated $\langle 0|s_i^z s_{i+1}^z|0 \rangle$ and plotted it versus $h$ (fig.5) which shows the
entrance to the SFM phase for $h > h_c(\Delta)$ in the $-1 \leq \Delta \leq 1$ region. It is an interesting
result which is obtained by a 3-sites block RG and can be compared with the exact result
\( h_c = \Delta + 1 \) [12]. Although the obtained critical value for \( h_c(\Delta) \) has a slight difference in the coefficients but preserves the linear form of the critical line. Our data for the ground state energy \( (e_o) \) show that \( h_c(\Delta) \) represents a critical line of 2nd order transition in which \( e_o \) and \( \frac{de_o}{dh} \) are continuous at \( h_c(\Delta) \) and is confirmed by the analytic results for \( e_o(h) \) at \( \Delta = 0 \) [17]. Our data along the \( \Delta = 0 \) and \( h = 0 \) lines recover the results of Drzewinski [11] and Rabin [16] respectively.

For the XXTF fixed point we have calculated the critical exponents which have been written in table-1. If \( R(h) \) represents the renormalization of \( h \) along the \( \Delta = 0 \) line the correlation length exponent \( (\nu) \) is given by \( \nu = \frac{\ln(n_B)}{\ln(R(h^*)))} \). The dynamical exponent \( (z) \) is \( z = \frac{\ln(n_B^* h^*)}{\ln(R(h^*))} \). The critical exponent \( \alpha \) connected with the specific heat is calculated from the hyper-scaling relation \( 2 - \alpha = d^* \nu \) [19], where \( d^* = d + z \) (\( d \) is the spatial dimension). The critical exponent \( \beta \), related to the magnetization is given by \( \beta = \frac{\ln(n_B^*)}{\ln(R(h^*))} \). These results show good agreement with the exact ones.

The other phase in the phase diagram is a classical anti-ferromagnetic phase. Let us first look at the exact solution of this model with the Hamiltonian as in eq.(12). By a simple argument we can find that the ground state is a Neel ordered state whose energy per site is \( \frac{E_n}{kn} = e_o = -\frac{1}{4} \) for \( 0 \leq g \leq 1 \) and is a saturated ferromagnetic state for \( g \geq 1 \) where \( e_o = \frac{1 - 2g}{4} \) (see appendix). These values for the ground state energy \( (e_o) \) show a discontinuity of \( \frac{de_o}{dg} \) at \( g = 1 \), which means the phase transition at this point is classified as a 1st order transition. By using the previous definitions for \( g = \frac{h}{\Delta} \), the RG–equations in (14) and (15) give a fixed point at \( g = 1 \) in the limit \( \Delta \to \infty \), which is equal to the exact critical point. The RG–flow in (14) and (15) show a fixed line at \( \Delta \to \infty \) for all \( g < 1 \). This means that there is a unique ground state for any value of \( 0 \leq g \leq 1 \) and the distinction between two different \( g \) values is only due to the excited states of the Hamiltonian.

We have also calculated the ground state energy by using the RG–equations (14) and (15) in a hierarchical way by accumulating the energies of the blocks (see appendix). The obtained result is equal to the exact result for the ground state energy.

\[
e_o = \begin{cases} 
\frac{-1}{4} & 0 \leq g \leq 1 \\
\frac{1 - 2g}{4} & g \geq 1
\end{cases}
\] (16)
Thus the limiting case of our RG–equations at $h, \Delta \gg 1$ exactly describe the classical anti-ferromagnetic Ising model.

There is an interesting point in the phase-diagram. When $-1 \leq \Delta \leq 1$ and $h < h_c(\Delta)$, the model represents a PM phase with $-0.5 < m \leq 0$ and undergoes a 2nd order transition to the SFM phase ($m = -0.5$) at $h_c(\Delta)$ ($m$ is continuous at the transition point). But at $h, \Delta \to \infty; \frac{h}{\Delta} < 1$ when the model represents a Neel ordered phase (AFI) with $m = 0$ and $sm = 0.5$, it undergoes a 1st order transition to the SFM phase ($m = -0.5$) at $h_c = \Delta$ ($m$ is discontinuous at the transition point). We have examined the continuity of the ground state energy and its derivatives up to the third order numerically at $\Delta = 1; h \neq 0$. Therefore there is a continuous change in the critical exponents by increasing $\Delta$ when $h < h_c$. This shows a crossover between PM and AFI phases. This change in the universality class is due to the reduction in the number of components of the spin operator (i.e. three components $s^x, s^y, s^z$ in the PM phase and effectively one component $s^z$ in the AFI phase). The crossover exponent $\phi = \frac{y_\Delta}{y_h}$ has been calculated to be 0.63 which verifies that the coupling $\Delta$ is relevant and causes crossover ($\lambda_i = n_{IB}^h$; where $\lambda_i$ is the eigenvalue at IAFH fixed point).

One can also retrieve the critical line $0 < \Delta < 1; h = 0$ by RSRG using the $su_q(2)$ symmetry of the xxz chain which differs only at the ends and is not important in the thermodynamic limit ($N \to \infty$). However it is not suitable for $\Delta > 1$ case and also in the presence of the external field ($h$) this RG prescription could not describe the critical line $h_c(\Delta)$.

5 Energy and Correlation Functions

In this section we describe some more results which have been obtained by RG–equations in section-3. In fig.3-a we have plotted the ground state energy per site ($e_o$) of the XX ($\Delta = 0$) model versus external magnetic field ($h$). We have also compared the RSRG results with the exact one[17]. In the PM phase (fig.3-a) there is a discontinuity in $e_o$ which is due to level crossing (finite size effects) of 3-sites block. This level crossing occurs as $h_0(\Delta = 0)$ passes the value 0.707. Thus we have not considered this point as a critical point. Fig.3-a shows good agreement with the exact results in the SFM phase ($h > h_c$) with a slight difference in
the PM phase. It has been shown\cite{6, 7, 8} that this difference is due to boundary conditions in an isolated block which neglects the remaining part of the chain. We have introduced a modified scheme to decrease this difference in the $h = 0$ case \cite{8}. By using the RG–equations of section-3 the ground state energy for different values of $\Delta$ can be calculated which will show the same behaviour as in fig.3. We have plotted the ground state energy for $\Delta = -1, -0.5, 0.5, 1$ cases in fig.3-b. The ground state energy at $\Delta = -1$ in fig.3-b confirms that the model represents the ferromagnetic Heisenberg model in the presence of an external magnetic field, where its ground state energy is proportional to the strength of the external field.

We have plotted in fig.4-a, the magnetization($m$) versus external magnetic field($h$) for $\Delta = 0$. It has been compared with the known exact result, which shows good agreement qualitatively. The step form of the RSRG results in this figure is due to the cyclic nature of the RG–equations in the PM phase. This is related to the nature of the anti-ferromagnetic problem. The magnetization curve reflects a continuous sequence of level-crossings between states with different values of the total $S_z$ induced by varying the magnetic field. The variational ground state which is obtained here is however owing to the highly degenerate energy level structure. The recurrence of this level crossing in the process of RG leads to the oscillatory behaviour of the RG flow. This oscillation is trapped by a metastable state which leads to a jump in the magnetization curve. Fig.4-a confirms that for $h < h_c$ the model is PM where $m \neq 0$ and reaches the SFM phase ($m = -0.5$) at $h = h_c$. We have also plotted the magnetization versus external field in fig.4-b for $\Delta = -0.5, 0.5$ and fig.4-c for $\Delta = 1.1, 1.5$ which show a similar behaviour as in the $\Delta = 0$ case, but the critical point where the model becomes SFM is different.

One of the important quantities which can be used to show the critical behaviour is the $z$–component of spin–spin correlation function. We have plotted $\langle 0|s^z_is^z_{i+1}|0 \rangle$ versus external magnetic field($h$) in fig.5 for different values of anisotropy parameter $\Delta$. Transition from the PM phase to the SFM phase occurs at two steps. The first jump is due to level crossing at $h_0(\Delta)$ which is not the critical point and does not terminate at the SFM phase. But the second jump which achieves the SFM phase ($\langle 0|s^z_is^z_{i+1}|0 \rangle = 0.25$), corresponds to the critical
point of the transition from the PM to the SFM phases. The location of critical point is at the same point in which the magnetization curves (fig.4-a, fig.4-b and fig.4-c) reaches the saturated value ($m = -0.5$). The critical point $h_c(\Delta)$ for different values of $\Delta$ which has been obtained in fig.5 yields the linear relation $h_c(\Delta) = 0.943\Delta + 0.943$. This result shows that RSRG is a good candidate to describe the critical behaviour of quantum systems[11].

We have also calculated the magnetization($m$) in the middle range $\Delta > 1$ and found that the critical line $h_c(\Delta) = 0.943\Delta + 0.943$ is also valid in this region. Since the RSRG method is an approximate scheme there is a small discrepancy between the obtained critical line and the exact one ($h_c = \Delta + 1$). This error is related to the small isolated blocks which are considered in this method. In other words the quantum fluctuations of a highly correlated system in a large lattice can not be simulated by a small number of eigenkets of an isolated block. However as $\Delta \to \infty$ and the model becomes classical one, exact results can be obtained by RSRG method (see appendix). This describes the discrepancy in the limit $\Delta \to \infty$ of $h_c(\Delta)$ which is $g_c = \frac{h_c}{\Delta} = 0.943 + O(1/\Delta)$ and $g_c = 1$ which can be obtained by RSRG method in the limit $\Delta \to \infty$ of the initial model. We have also calculated the z-component of spin–spin correlation function in terms of distance. In fig.6 we have plotted $\langle s_i^z s_{i+r}^z \rangle$ at $\Delta = 1$ for different values of $h$ below and above its critical point($h_c = 1.886$). When $h = 0$, the correlation length is small(in the order of lattice spacing) and the correlation function goes rapidly to zero after a few lattice spacing. As $h$ increases to its critical value the correlation function becomes nonzero for long distances and shows exactly the SFM phase above the critical point($h > h_c$). The same behaviour has also been observed for other values of the anisotropy parameter $\Delta$.

6 Conclusion

We have considered the anisotropic anti-ferromagnetic Heisenberg chain in the presence of an external magnetic field by RSRG. We have sketched the phase diagram of this model for $\Delta \geq -1$ and $h > 0$ in fig.2, the phase diagram for $\Delta \geq -1$ and $h < 0$ is the mirror image of the previous case. We have obtained three distinct phases in the phase diagram. The partially magnetized (PM) phase with $m \neq 0$, the saturated ferromagnetic (SFM)
phase with \( m = -0.5 \) and the Neel ordered phase (AFI) where \( m = 0 \). By computing the magnetization and the z-component of spin-spin correlation function we have calculated the critical line \( h_c(\Delta) = 0.943\Delta + 0.943 \) between the PM and SFM phases which causes a 2nd order transition. But at \( \Delta \to \infty \) the transition from AFI to SFM phases is 1st order at the critical point \( g_c = 1 \). We have observed that for \( h < h_c \) increasing \( \Delta \) causes a crossover between PM and AFI phases which changes the universality class of the model. The crossover exponent has been calculated to be \( \phi = 0.63 \) which confirms the relevance of the anisotropy \( \Delta \) in the crossover phenomena.

By using the analytical RG–equations we have obtained the critical exponents at the XXTF fixed point. Although the obtained critical exponents are not accurate compared with the exact results they show good agreement with them. The ground state energy and correlation functions calculated in the PM phase, show qualitatively good results, but some discrepancy due to the boundary conditions of the isolated block in the RG procedure is present. However all the results in the SFM phase are completely accurate, because the ground state of the whole chain in this phase is a simple juxtaposition of the ground state of the isolated blocks and there is not any boundary condition effects for an isolated block as in the PM phase. In the AFI fixed point when the model is a classical one, the limiting form of our analytical RG–equations \( (\Delta \to \infty) \) give the exact results for the ground state energy and the critical point \( g_c = 1 \). We have shown that the critical line \( h_c(\Delta) \) is also valid in the middle range \( \Delta > 1 \). Finally we conclude that the standard quantum RG (RSRG) gives qualitatively good results for the critical behaviour of the system. However the quantitative results for the location of the critical point and critical exponents is much better than its results for ground state energy and correlation functions with respect to the known exact results.

7 Acknowledgement

I would like to express my deep gratitude to V. Karimipour and J. Davoodi for valuable comments and discussions and M.A. Martin-Delgado for a careful study of the manuscript and very useful comments. Interesting conversations with B.Davoodi, M.R.Ejtehadi, M. R.
Rahimi-Tabar, K. Kaviani, R. Razmi and M. Abolfath are also acknowledged.

8 Appendix: Classical anti-ferromagnetic Ising model in an external field

8.1 Exact ground state

The classical anti-ferromagnetic Ising model in the presence of an external magnetic field is given by equation (12)

\[ H_{AFI} = k \sum_{i=1}^{N} (s_i^z s_{i+1}^z + gs_i^z) \]

where \( k = J \Delta > 0 \) and \( g = \frac{h}{\Delta} \) is the strength of external magnetic field. We assume periodic boundary condition \( s_{N+1}^z = s_1^z \). Let us write the Hamiltonian in terms of Pauli matrices,

\[ H_{AFI} = \frac{k}{4} \sum_{i=1}^{N} (\sigma_i^z \sigma_{i+1}^z - 1) + 2g \sum_{i=1}^{N} \sigma_i^z + N. \]  

(17)

The energy \( E \) of this chain is

\[ E = \frac{k}{4} [-2n_f + 2gn_s + N], \]  

(18)

where \( n_s = n_p - n_m \), \( n_p \) is the number of up spins, \( n_m \) is the number of down spins \( (n_p + n_m = N) \) and \( n_f \) is the number of boundary walls of flipped spins. The maximum value of \( n_f \) is obtained by a Neel ordered state \( n_p = n_m = \frac{N}{2}, n_f = N \), but for an arbitrary value of \( n_s \) it can be written as

\[ (n_f)_{max} = N - |n_s|. \]  

(19)

By using the definition of \( n_s \), \( (n_f)_{max} \) can be written in the following form

\[ (n_f)_{max} = N - |N - 2n_m| = \begin{cases} 2n_m & n_m \leq \frac{N}{2} \\ 2(N - n_m) & n_m \geq \frac{N}{2} \end{cases} \]  

(20)

The minimum value of \( E \) will be obtained if \( n_s \) has its minimum value and \( n_f \) has its maximum value.

\[ E_o = \min(E) = \frac{k}{4} [N + 2g(N - 2n_m) - 2(n_f)_{max}]. \]  

(21)
When \( n_m \leq \frac{N}{2} \), we have \( \frac{E_{o}^N}{kN} = e_o = \frac{-1}{4} \) which is greater than all the energies in the \( n_m \geq \frac{N}{2} \) case. Therefore we will investigate \( E_o \) in the \( n_m \geq \frac{N}{2} \) region by minimizing \( E \) with respect to \( n_m \), which is

\[
e_o = \begin{cases} 
\frac{-1}{4} & g \leq 1 \ (n_m = \frac{N}{2}) \\
\frac{1-2g}{4} & g \geq 1 \ (n_m = N)
\end{cases}
\]

It is obvious from (22) that for any value of \( g \leq 1 \) the ground state energy is due to a Neel ordered state \( (n_m = \frac{N}{2}, n_f = N) \) and for \( g \geq 1 \) the ground state is a saturated ferromagnetic state \( (n_m = N, n_f = 0) \).

8.2 Renormalization group equations

At large \( \Delta (\Delta \rightarrow \infty) \), the renormalization group equations (14) and (15) can be written for \( k = J\Delta > 0 \) and \( g = \frac{k}{\Delta} \geq 0 \) in the following form

\[
g < 1 : \quad \begin{cases} 
k' = k, \\
g' = g,
\end{cases}
\]

\[
g > 1 : \quad \begin{cases} 
k' = b^2k; \\
g' = \frac{1}{g}(g - 1).
\end{cases}
\]

The RG equations in (23) give no running of coupling constants and lead to a fixed line \( 0 \leq g \leq 1 \). As far as the ground state energy is concerned, there is no distinction between any arbitrary value of \( 0 \leq g \leq 1 \). But when \( g > 1 \) the only fixed point is \( g^* = 1 \) which is at the end of the fixed line \( 0 \leq g \leq 1 \). Thus \( g^* = 1 \) is the critical value of \( g \) which separates the \( g < 1 \) and \( g > 1 \) phases. To be more rigorous and define these phases we will calculate the magnetization \( (m) \) and staggered magnetization \( (sm) \) in these regions. Equations (8) and (9) in the limit \( \Delta \rightarrow \infty (a \rightarrow 1, b \rightarrow 0) \) will be written as

\[
g < 1 : \quad T_s^{z}T = s^{z} ; \quad T_{s}^{\dagger}s^{z}T = -s^{z}
\]

\[
g > 1 : \quad T_s^{z}T = \frac{-i}{2} ; \quad T_{s}^{\dagger}s^{z}T = s^{z}.
\]

The magnetization \( (m = \frac{1}{N} \sum^N_i \langle s_i^z |0\rangle) \) is

\[
m = \frac{1}{N} \sum_{\mu=1}^{N/3} \langle 0|(s_{1\mu} + s_{2\mu} + s_{3\mu})|0\rangle
\]
\[
\frac{1}{N} \sum_{\mu=1}^{N/3} \langle 0 | T^\dagger (s_{1\mu}^z + s_{2\mu}^z + s_{3\mu}^z) T | 0' \rangle
\]

where \(|0'\rangle\) is the ground state in the renormalized Hilbert space \((T|0'\rangle = |0\rangle)\). By using equation (27), the magnetization is calculated to be

\[
m = \frac{1}{3} m' \quad ; \quad g < 1
\]

\[
m = -\frac{1}{3} + \frac{1}{3} m' \quad ; \quad g > 1
\]

where \(m'\) is the magnetization in the renormalized chain with \(N/3\) sites. However in the thermodynamic limit \((N \to \infty)\), \(m\) and \(m'\) will be equal. Thus equation (27) gives

\[
m = 0 \quad ; \quad g < 1
\]

\[
m = -0.5 \quad ; \quad g > 1.
\]

Similarly, we can use the definition of staggered magnetization

\[
sm = \frac{1}{N} \sum_i N/3 \langle 0 | (-1)^i s_i^z | 0 \rangle
\]

and repeat the steps in calculating \(m\), the staggered magnetization is obtained to be

\[
sm = 0.5 \quad ; \quad g < 1
\]

\[
sm = 0 \quad ; \quad g > 1.
\]

These results confirm the Neel ordered state in the \(g < 1\) region and the saturated ferromagnetic state in the \(g > 1\). Note that these results are the same as the exact ones which have been obtained in the last section. Had we taken even size blocks for the renormalization procedure, we could not obtain these values.

The calculation of the ground state energy is easily done by accumulating the energy of blocks in a hierarchical way. The renormalized Hamiltonian is

\[
H^{'(k,g')}_{\frac{3}{2}}(k',g') = T^\dagger H_N(k,g) T = \begin{cases} \frac{k}{4}(\frac{2N}{3}) + k \frac{N/3}{i} s_i^z s_{i+1}^z + g s_i^z \quad ; \quad g < 1 \\ \frac{kN}{(1-4g)} + k(g - 1) \frac{N/3}{i} s_i^z \quad ; \quad g > 1 \end{cases}
\]

Therefore the ground state energy per site is calculated to be

\[
e_o = \frac{E_o}{kN} = \begin{cases} \frac{1}{4}(\frac{2}{3})(1 + \frac{1}{3} + \frac{1}{9} + ...) = \frac{-1}{4} \quad ; \quad g < 1 \\ \frac{1-4g}{12} - \frac{2(g-1)}{12} = \frac{1-2g}{4} \quad ; \quad g > 1 \end{cases}
\]

which is equal to the exact ground state energy. This result can not be either obtained by taking an even size block in the RG procedure.
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## Tables

Table-1. Eigenvalues and critical exponents at the XXTF fixed point, both RSRG and exact results.

|       | $\lambda_1$ | $\lambda_2$ | $\beta$  | $\nu$  | $z$  | $\alpha$ |
|-------|--------------|--------------|----------|--------|------|----------|
| RSRG  | 0.250        | 4.000        | 0.792    | 0.792  | 1.262| 0.208    |
| Exact | –            | –            | 0.5      | 0.5    | 2    | 0.5      |
**Figure Captions:**

**Fig.1)** Decomposition of lattice into block and inter–block part, and different types of intra–block ($H^B$) and inter–block ($H^{BB}$) interactions.

**Fig.2)** Phase diagram of the $xxz$ model in the presence of an external magnetic field ($h$). Filled circles are the fixed points and arrows show the direction of flow. The solid line which passes through the $(\Delta = -1, h = 0)$ and $(\Delta = 1, h = 1.886)$ points is the critical line $h_c = 0.943\Delta + 0.943$. The dotted line for $\Delta > 1$ shows qualitatively the crossover region. The double solid line at $\Delta = \infty$ is the fixed line $0 < g \leq 1$.

**Fig.3-a)** Ground state energy per site versus external field ($h$) for $\Delta = 0$, both RSRG and exact results.

**Fig.3-b)** Ground state energy per site versus external field ($h$) for $\Delta = -1, -0.5, 0.5, 1$, which has been obtained by RSRG.

**Fig.4-a)** Magnetization ($m = \frac{1}{N} \sum_{i=1}^{N} \langle 0 | s^z_i | 0 \rangle$) versus external field ($h$) for $\Delta = 0$, both RSRG and exact results.

**Fig.4-b)** Magnetization ($m = \frac{1}{N} \sum_{i=1}^{N} \langle 0 | s^z_i | 0 \rangle$) versus external field ($h$) for $\Delta = -0.5, 0.5$, which has been obtained by RSRG.

**Fig.4-c)** Magnetization ($m = \frac{1}{N} \sum_{i=1}^{N} \langle 0 | s^z_i | 0 \rangle$) versus external field ($h$) for $\Delta = 1.1, 1.5$, which has been obtained by RSRG.

**Fig.5)** $z$–component of spin–spin correlation function for different value of anisotropy parameter ($\Delta$) versus external field ($h$).

**Fig.6)** $z$–component of spin–spin correlation function at $\Delta = 1$ versus distance ($r$) for different value of external field ($h$).
$H = H^B + H^{BB}$

On-site interaction

Nearest neighbour interaction

Figure 1
Figure 2
Figure 3-a: Ground State Energy vs. External Field (h)

- RSRG
- Exact

(Δ=0)
Figure. 3-b

Ground State Energy vs. External Field (h)

- $\Delta = 1$
- $\Delta = 0.5$
- $\Delta = -0.5$
- $\Delta = -1$
Figure 4-b
Figure 4-c
$\Delta = 10.70.30-0.7-0.3$

Figure. 5
Figure 6