Phase diagram of the antiferromagnetic *XXZ* model in the presence of an external magnetic field

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(Received 4 May 1998; revised manuscript received 23 July 1998)

The anisotropic $s=\frac{1}{2}$ antiferromagnetic Heisenberg chain in the presence of an external magnetic field is studied by using the standard quantum renormalization group (RG). We obtain the critical line of the transition from the partially magnetized (PM) phase to the saturated ferromagnetic phase. The crossover exponent between the PM phase and antiferromagnetic Ising phase is evaluated. Our results show that the anisotropy (Δ) 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.
[S0163-1829(98)09141-3]

I. 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 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 behavior of the systems. The study of the ground state and its energy is thus of centeral importance for understanding the critical behavior of such systems.

The technique of the renormalization group (RG) has been so devised to deal with these multiscale problems.[1–4] In the momentum space RG which is suitable for studying continuous systems one iteratively integrates out 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 sites of the new lattice.[5] The Hamiltonian is divided into intrablock and interblock 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 is especially sensitive to the boundary conditions[6–8] which are considered for the block Hamiltonian. The detailed form of this projection in fact differentiates various versions of the real space (RS) RG, ranging from the standard RG to the recent density matrix RG (DMRG).[9] Each of these versions has its own advantages and disadvantages.

The Ising model in a transverse field (ITF) and anisotropic *XY* model in a transverse field (AXYTF) have been studied in Refs. 10 and 11 using both standard RG and DMRG methods. There, it has been concluded that the 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 is not low 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 behavior 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 behaviors. In this study we have succeeded in obtaining the critical line between the partially magnetized (PM) and saturated ferromagnetic (SFM) phases, to good accuracy, compared with the known results.[12] We have also derived the crossover between the PM phase (small anisotropy $-1<\Delta<1$) and the antiferromagnetic Ising (AFI) phase (large anisotropy $\Delta\gg 1$) 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 the RSRG is a good candidate to study at least the qualitative behavior of quantum lattice systems in the quantum critical region.

In this paper we have studied the $XXZ+H$ model by the RSRG method where the block length is 3 ($n_B=3$). In the next section we will introduce the $XXZ+H$ model and discuss its critical behavior as derived by other methods. In Sec. III we will discuss 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 behavior of the $XXZ+H$ model by RG equations in Sec. IV. In Sec. V 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.

II. MODEL

The anisotropic spin-$\frac{1}{2}$ antiferromagnetic 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.[12–14] 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,[15] where the critical fluctuations along the critical line are governed by a conformal field theory with central charge $c=1$. A RG study of the *XXZ* model has been performed by Rabin.[16] At $\Delta=0$, even in the presence of a magnetic field, the model can be mapped by a 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

$$H(J,\Delta,h)=J\sum_{i=1}^{N}(s_i^x s_{i+1}^x+s_i^y s_{i+1}^y+\Delta s_i^z s_{i+1}^z+hs_i^z), \quad (1)$$

where $J>0$, Δ is the anisotropy parameter, which in the antiferromagnetic 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 *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] A 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 $U=\exp(i\pi\Sigma_{j=1}^{N}js_j^z)$ 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 $\mathrm{su}_q(2)$.[18] If $h\neq 0$, the only symmetry is U(1). Let us now begin the RG study of the *XXZ+H* model.

III. RENORMALIZATION GROUP EQUATIONS

The implementation of the RSRG is based on two important points, the size of blocks and the number of states kept in each step of the RG. Both of them would have significant effects on the RG flow. Here we choose a three-site 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 Δ 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 later; see also the Appendix). Finally taking larger blocks renders an analytic RG equation difficult to obtain.

After dividing the whole chain into three-site blocks, the first step of the RSRG is to divide the Hamiltonian into two parts, the intrablock Hamiltonian (H^B) and the interblock 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

$$H_\mu^B=J[s_1^x s_2^x+s_2^x s_3^x+s_1^y s_2^y+s_2^y s_3^y+\Delta(s_1^z s_2^z+s_2^z s_3^z)+h(s_1^z+s_2^z+s_3^z)], \quad (2)$$

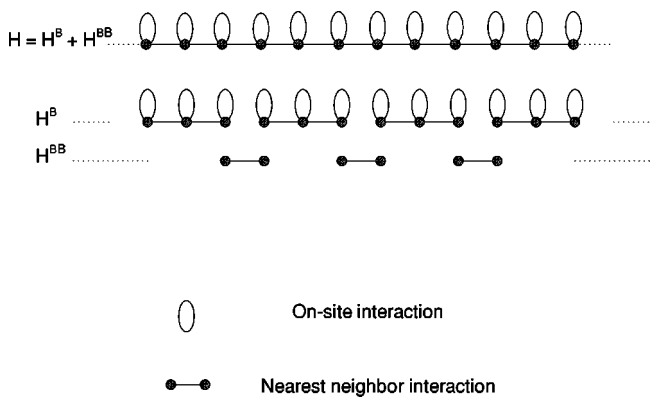


FIG. 1. Decomposition of the lattice into block and interblock parts, and different types of intrablock (H^B) and interblock (H^{BB}) interactions.

where μ represents the block number, i.e., $H^B=\Sigma_{\mu=1}^{N/3}H_\mu^B$. 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

$$T=|\alpha\rangle\langle+|+|\beta\rangle\langle-|, \quad (3)$$

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_μ^B, 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 three-site block and reaches the critical value of an 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 a 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 $h<h_0$,

$$|\alpha\rangle=b|++-\rangle+a|+-+\rangle+b|-++\rangle,$$
$$|\beta\rangle=-b|--+\rangle-a|-+-\rangle-b|+--\rangle, \quad (4)$$

where

$$h_0(\Delta)=\frac{3\Delta+\sqrt{\Delta^2+8}}{4},$$
$$a=\frac{2x+2}{\sqrt{6+12x^2}},\quad b=\frac{2x-1}{\sqrt{6+12x^2}}, \quad (5)$$

and

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

for $h>h_0$,

$$|\alpha\rangle=-b|--+\rangle-a|-+-\rangle-b|+--\rangle,$$
$$|\beta\rangle=|---\rangle. \tag{6}$$

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

$$O'=T^{\dagger}OT. \tag{7}$$

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

$$T^{\dagger}s^x_{1(3)}T=-2abs'^x, \quad T^{\dagger}s^x_2T=-2b^2s'^x,$$
$$T^{\dagger}s^y_{1(3)}T=2abs'^y, \quad T^{\dagger}s^y_2T=2b^2s'^y, \tag{8}$$
$$T^{\dagger}s^z_{1(3)}T=a^2s'^z, \quad T^{\dagger}s^z_2T=(1-2a^2)s'^z.$$

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

$$T^{\dagger}s^x_{1(3)}T=-bs'^x, \quad T^{\dagger}s^x_2T=-as'^x,$$
$$T^{\dagger}s^y_{1(3)}T=bs'^y, \quad T^{\dagger}s^y_2T=as'^y,$$
$$T^{\dagger}s^z_{1(3)}T=-\frac{a^2+1}{4}I+\frac{1-a^2}{2}s'^z,$$
$$T^{\dagger}s^z_2T=\frac{a^2-1}{2}I+a^2s'^z. \tag{9}$$

In the above equations s'^{α} 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 Eqs. (8) and (9) we will obtain the renormalization of coupling constants in the Hamiltonian: for $|h|<h_0(\Delta)$,

$$J'=4a^2b^2J,$$
$$\Delta'=\frac{a^2}{4b^2}\Delta,$$
$$h'=\frac{1}{4a^2b^2}h; \tag{10}$$

for $|h|>h_0(\Delta)$,

$$J'=b^2J,$$
$$\Delta'=b^2\Delta,$$
$$h'=\frac{1}{b^2}\left(|h|-h_0+\frac{a^4-1}{4}\Delta\right)\mathrm{sgn}(h). \tag{11}$$

The above RG equations show that the renormalized Hamiltonian is of the same form as the original one. The critical behavior which can be obtained from these equations will be discussed in the next section.

Let us consider an extreme case where both h and Δ go to infinity and J goes to zero such that $J\Delta$, Jh, and h/Δ remain finite. In this case the Hamiltonian reduces to a simple antiferromagnetic Ising model in the presence of an external magnetic field, which shows a first-order transition from a classical antiferromagnetic (Néel) ordered phase [$m=0, sm=(1/N)\Sigma_i(-1)^i s^z_i=0.5$] to a saturated ferromagnetic phase ($|m|=0.5, sm=0$). We can write this Hamiltonian as

$$H_{AFI}=k\sum_i (s^z_is^z_{i+1}+gs^z_i), \tag{12}$$

where

$$k=J\Delta>0, \quad g=\frac{h}{\Delta}. \tag{13}$$

At large Δ ($\Delta\gg1$) we have $h_0\simeq\Delta$, $a\to1$, and $b\to0$. Then the RG equations reduce to the following equations: for $|h|<\Delta$,

$$J'=4b^2J,$$
$$\Delta'=\frac{1}{4b^2}\Delta,$$
$$h'=\frac{1}{4b^2}h; \tag{14}$$

for $|h|>\Delta$,

$$J'=b^2J,$$
$$\Delta'=b^2\Delta,$$
$$h'=\frac{1}{b^2}(|h|-\Delta)\mathrm{sgn}(h). \tag{15}$$

These RG equations give exactly the critical point $g_c=1$ and the ground state energy of the AFI model (see the Appendix), which will be discussed in the next section.

IV. CRITICAL BEHAVIOR

In this section we analyze the RG equations and their critical behavior. The phase diagram of the obtained RG flow [Eqs. (10) and (11)] is depicted in Fig. 2. This phase diagram consists of three different phases, partially magnetized, classical antiferromagnetic, and saturated ferromagnetic phases.

There are five fixed points in the phase diagram.

(i) XX represents a spin-$\frac{1}{2}$ *XX* model without an 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 antiferromagnetic Ising model with a long-range Néel order.

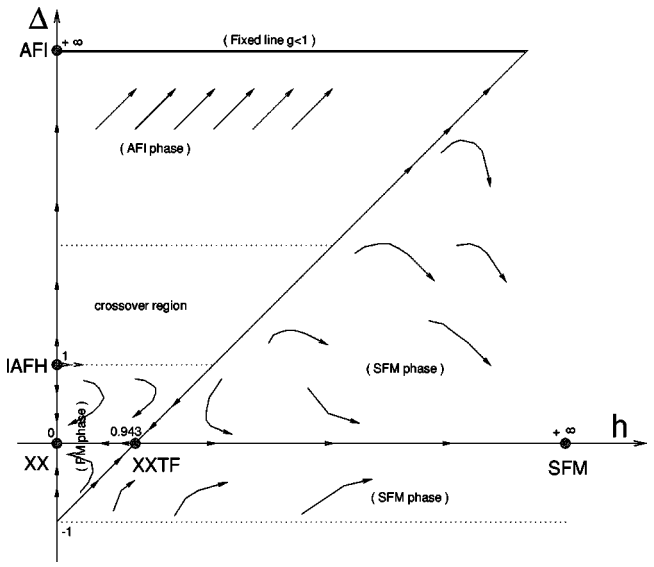


FIG. 2. Phase diagram of the *XXZ* model in the presence of an external magnetic field (h). Solid circles are the fixed points and arrows show the direction of flow. The solid line which passes through the ($\Delta=-1,h=0$) and ($\Delta=1,h=1.886$) points is the critical line $h_c=0.943\Delta+0.943$.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

(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 behavior and goes to the SFM fixed point for any value of $h>h_c(\Delta)$. But when $h<h_c(\Delta)$ and $-1\leqslant\Delta\leqslant 1$ 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 the RG leads to the oscillatory behavior of the RG flow. If we imagine a three-dimensional RG flow, its projection onto the h-Δ 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 I, 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 behavior 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 $-1\leqslant\Delta\leqslant 1$ region. It is an interesting result which is obtained by a three-site 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_0) show that $h_c(\Delta)$ represents a critical line of a second-order transition in which e_0 and de_0/dh are continuous at $h_c(\Delta)$, which is confirmed by the analytic results for $e_0(h)$ at $\Delta=0$.[17] Our results along the $\Delta=0$ and $h=0$ lines recover the results of Drzewinski and Dekeyser[11] and Rabin,[16] respectively.

TABLE I. Eigenvalues and critical exponents at the XXTF fixed point, both RSRG and exact results.

	λ_1	λ_2	β	ν	z	α
RSRG	0.250	4.000	0.792	0.792	1.262	0.208
Exact	-	-	0.5	0.5	2	0.5

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

The other phase in the phase diagram is a classical antiferromagnetic 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 Néel ordered state whose energy per site is $E_0/kN=e_0=-\frac{1}{4}$ for $0\leqslant g\leqslant 1$ and is a saturated ferromagnetic state for $g\geqslant 1$ where $e_0=(1-2g)/4$ (see the Appendix). These values for the ground state energy (e_0) show a discontinuity of de/dg at $g=1$, which means the phase transition at this point is classified as a first-order transition. By using the previous definitions for $g=h/\Delta$, the RG equations (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 Eqs. (14) and (15) shows a fixed line at $\Delta\to\infty$ for all $g<1$. This means that there is a unique ground state for any value of $0\leqslant g\leqslant 1$ 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 the Appendix). The obtained result is equal to the exact result for the ground state energy:

$$e_0=\begin{cases} -\dfrac{1}{4}, & 0\leqslant g\leqslant 1, \\ \dfrac{1-2g}{4}, & g\geqslant 1. \end{cases} \tag{16}$$

Thus the limiting case of our RG equations at $h,\Delta\gg 1$ exactly describes the classical antiferromagnetic Ising model.

There is an interesting point in the phase diagram. When $-1\leqslant\Delta\leqslant 1$ and $h<h_c(\Delta)$, the model represents a PM phase with $-0.5<m\leqslant 0$ and undergoes a second-order transition to the SFM phase ($m=-0.5$) at $h_c(\Delta)$ (m is continuous at the transition point). But at $h,\Delta\to\infty, h/\Delta<1$ when the model represents a Néel ordered phase (AFI) with $m=0$ and $sm=0.5$, it undergoes a first-order transition to the SFM phase ($m=-0.5$) at $h_c=\Delta$ (m is discontinuous at the tran-

sition point). We have examined the continuity of the ground state energy and its derivatives up to third order numerically at $\Delta=1, h\neq 0$. Therefore there is a continuous change in the critical exponents by increasing Δ 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 $\phi = y_\Delta / y_h$ has been calculated to be 0.63 which verifies that the coupling Δ is relevant and causes crossover ($\lambda_i = n_B^{y_i}$, where λ_i is the eigenvalue at IAFH fixed point).

One can also retrieve the critical line $0<\Delta<1$, $h=0$ by the RSRG using the $su_q(2)$ symmetry[20] 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 the $\Delta>1$ case and also in the presence of the external field (h) this RG prescription could not describe the critical line $h_c(\Delta)$.

V. ENERGY AND CORRELATION FUNCTIONS

In this section we describe some more results which have been obtained by RG equations in Sec. III. In Fig. 3(a) we have plotted the ground state energy per site (e_0) 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_0 which is due to the level crossing (finite size effects) of a three-site 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. Figure 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[6–8] 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.[8] By using the RG equations of Sec. III the ground state energy for different values of Δ can be calculated which will show the same behavior 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 antiferromagnetic problem. The magnetization curve reflects a continuous sequence of level crossings between states with different values of 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 behavior of the RG flow. This oscillation is trapped by a metastable state which leads to a jump in the magnetization curve. Figure 4(a) confirms that for $h<h_c$ the

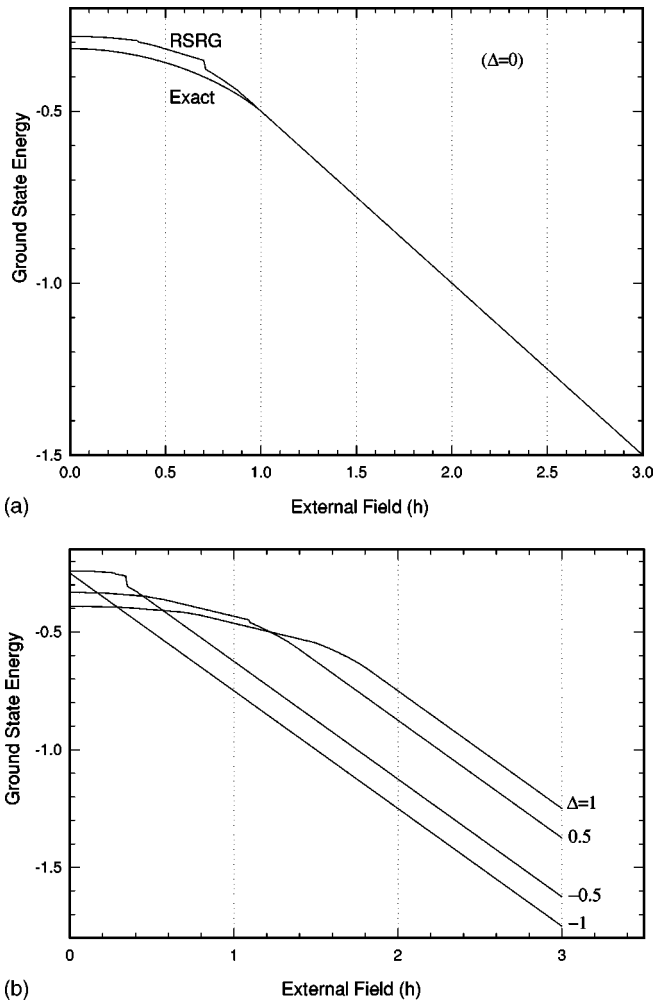
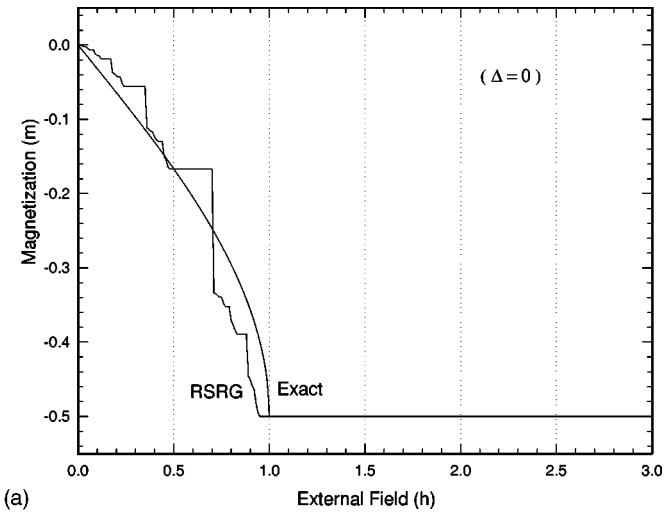
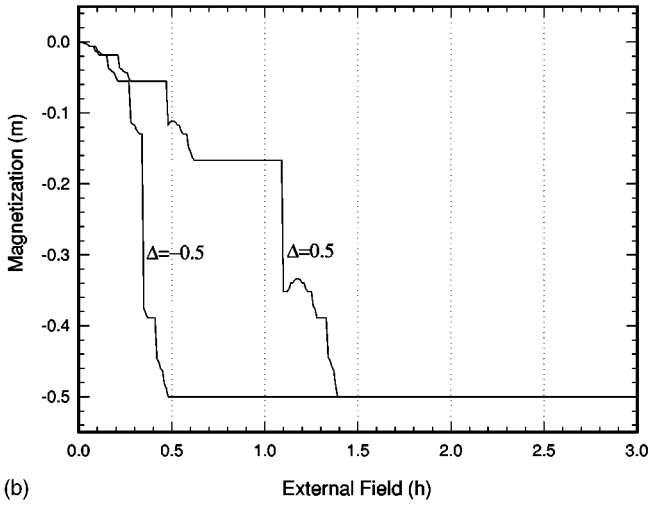


FIG. 3. (a) Ground state energy per site vs external field (h) for $\Delta=0$, both RSRG and exact results. (b) Ground state energy per site vs external field (h) for $\Delta=-1, -0.5, 0.5, 1$, which has been obtained by the RSRG.

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 in Fig. 4(c) for $\Delta=1.1, 1.5$ which show a similar behavior 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 behavior is the z component of the spin-spin correlation function. We have plotted $\langle 0|s_i^z s_{i+1}^z|0\rangle$ versus external magnetic field (h) in Fig. 5 for different values of the anisotropy parameter Δ. The transition from the PM phase to the SFM phase occurs in 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 ($\langle 0|s_i^z s_{i+1}^z|0\rangle = 0.25$), corresponds to the critical point of the transition from the PM to the SFM phases. The location of the critical point is at the same point in which the magnetization curves [Figs. 4(a), 4(b), and 4(c)] reaches the saturated value ($m=-0.5$). The critical point $h_c(\Delta)$ for different values of Δ which has been obtained in Fig. 5 yields the linear relation $h_c(\Delta)=0.943\Delta + 0.943$. This result shows that the RSRG is a good candidate to describe the critical behavior of quantum systems.[11]





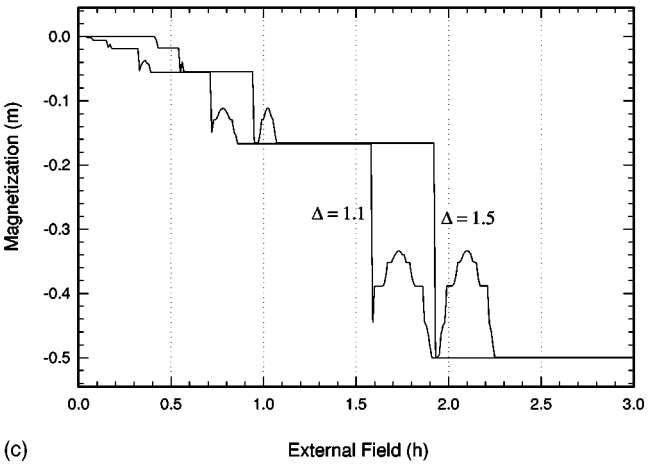


FIG. 4. (a) Magnetization $[m=(1/N)\,\Sigma_{i=1}^{N}\langle 0|s_i^z|0\rangle]$ vs external field (h) for $\Delta=0$, both RSRG and exact results. (b) Magnetization $[m=(1/N)\,\Sigma_{i=1}^{N}\langle 0|s_i^z|0\rangle]$ vs external field (h) for $\Delta=-0.5$, 0.5, which has been obtained by the RSRG. (c) Magnetization $[m=(1/N)\,\Sigma_{i=1}^{N}\langle 0|s_i^z|0\rangle]$ vs external field (h) for $\Delta=1.1$, 1.5, which has been obtained by the RSRG.

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 cannot be simulated by a small number of eigenkets of an isolated block. However, as $\Delta\to\infty$ and the model becomes a classical one, exact results can be obtained by the RSRG method (see the Appendix). This describes the discrepancy in the limit $\Delta\to\infty$ of $h_c(\Delta)$ which is $g_c=h_c/\Delta=0.943+O(1/\Delta)$ and $g_c=1$ which can be obtained by the RSRG method in the limit $\Delta\to\infty$ of the initial model. We have also calculated the z component of the spin-spin correlation function in terms of distance. In Fig. 6 we have plotted $\langle 0|s_i^z s_{i+r}^z|0\rangle$ 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 the lattice spacing) and the correlation function goes rapidly to zero after a few lattice spacings. As h increases to its critical value the correla-

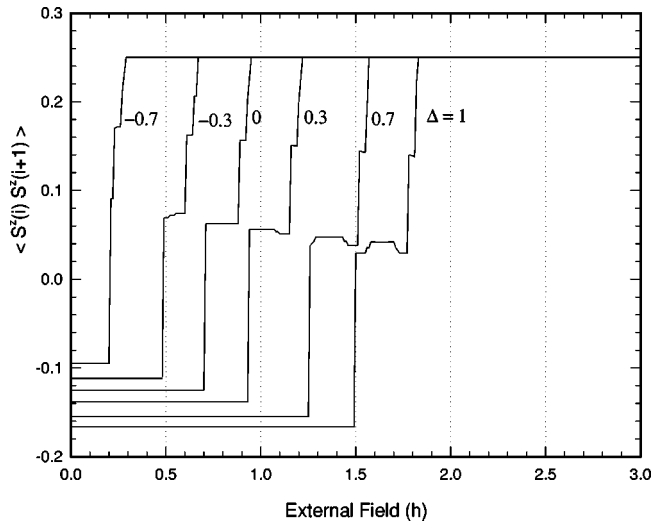


FIG. 5. z component of the spin-spin correlation function for different values of the anisotropy parameter (Δ) vs external field (h).

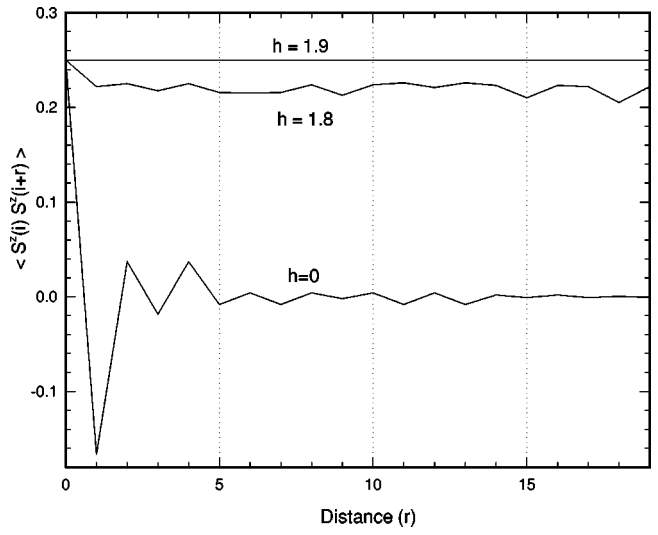


FIG. 6. z component of the spin-spin correlation function at $\Delta=1$ vs distance $(\mathbf{r})$ for different values of the external field (h).

tion function becomes nonzero for long distances and shows exactly the SFM phase above the critical point ($h>h_c$). The same behavior has also been observed for other values of the anisotropy parameter Δ.

VI. CONCLUSION

We have considered the anisotropic antiferromagnetic Heisenberg chain in the presence of an external magnetic field by the RSRG. We have sketched the phase diagram of this model for $\Delta \geqslant -1$ and $h>0$ in Fig. 2, the phase diagram for $\Delta \geqslant -1$, and $h<0$ is the mirror image of the previous case. We have obtained three distinct phases in the phase diagram. The partially magnetized phase with $m \neq 0$, the saturated ferromagnetic phase with $m=-0.5$, and the Néel ordered phase (AFI) where $m=0$. By computing the magnetization and the z component of the 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 second-order transition. But at $\Delta \to \infty$ the transition from AFI to SFM phases is first order at the critical point $g_c=1$. We have observed that for $h<h_c$ increasing Δ 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 Δ in the crossover phenomena.

By using 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 are no 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 ($\Delta \to \infty$) gives 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 behavior of the system. However, the quantitative results for the location of the critical point and critical exponents are much better than the results for the ground state energy and correlation functions with respect to the known exact results.

ACKNOWLEDGMENTS

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.

APPENDIX: CLASSICAL ANTIFERROMAGNETIC ISING MODEL IN AN EXTERNAL FIELD

1. Exact ground state

The classical antiferromagnetic Ising model in the presence of an external magnetic field is given by Eq. (12):

$$H_{AFI}=k\sum_{i=1}^{N}(s_i^z s_{i+1}^z + g s_i^z),$$

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

$$H_{AFI}=\frac{k}{4}\left[\sum_{i=1}^{N}(\sigma_i^z\sigma_{i+1}^z-1)+2g\sum_{i=1}^{N}\sigma_i^z+N\right]. \quad \text{(A1)}$$

The energy (E) of this chain is

$$E=\frac{k}{4}[-2n_f+2gn_s+N], \quad \text{(A2)}$$

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 Néel ordered state ($n_p=n_m=N/2, n_f=N$), but for an arbitrary value of n_s it can be written as

$$(n_f)_{max}=N-|n_s|. \quad \text{(A3)}$$

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

$$(n_f)_{max}=N-|N-2n_m|=\begin{cases} 2n_m, & n_m \leqslant \dfrac{N}{2}, \\ 2(N-n_m), & n_m \geqslant \dfrac{N}{2}. \end{cases} \quad \text{(A4)}$$

The minimum value of E will be obtained if n_s has its minimum value and n_f has its maximum value:

$$E_0=\min(E)=\frac{k}{4}[N+2g(N-2n_m)-2(n_f)_{\max}]. \quad \text{(A5)}$$

When $n_m \leqslant N/2$, we have $E_0/kN=e_0=-1/4$ which is greater than all the energies in the $n_m \geqslant N/2$ case. Therefore we will investigate E_0 in the $n_m \geqslant N/2$ region by minimizing E with respect to n_m, which is

$$e_0=\begin{cases} -\dfrac{1}{4}, & g \leqslant 1 \quad \left(n_m=\dfrac{N}{2}\right), \\ \dfrac{1-2g}{4} & g \geqslant 1 \quad (n_m=N). \end{cases} \quad \text{(A6)}$$

It is obvious from Eq. (A6) that for any value of $g \leqslant 1$ the ground state energy is due to a Néel ordered state ($n_m=N/2, n_f=N$) and for $g \geqslant 1$ the ground state is a saturated ferromagnetic state ($n_m=N, n_f=0$).

2. Renormalization group equations

At large $\Delta(\Delta\to\infty)$, the renormalization group equations (14) and (15) can be written for $k=J\Delta>0$ and $g=h/\Delta \geqslant 0$ in the following form: for $g<1$,

$$k'=k,$$

$$g'=g; \tag{A7}$$

for $g>1$,

$$k'=b^4k,$$

$$g'=\frac{1}{b^4}(g-1). \tag{A8}$$

The RG equations (A7) give no running of the coupling constants and lead to a fixed line $0\leqslant g\leqslant 1$. As far as the ground state energy is concerned, there is no distinction between any arbitrary value of $0\leqslant g\leqslant 1$. But when $g>1$ the only fixed point is $g^*=1$ which is at the end of the fixed line $0\leqslant g \leqslant 1$. 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 $\Delta\to\infty$ ($a\to 1, b\to 0$) will be written as

$$g<1, \quad T^\dagger s^z_{1(3)}T=s'^z, \quad T^\dagger s^z_2 T=-s'^z,$$

$$g>1, \quad T^\dagger s^z_{1(3)}T=\frac{-I}{2}, \quad T^\dagger s^z_2 T=s'^z. \tag{A9}$$

The magnetization $[m=(1/N)\,\Sigma_i^N\langle 0|s_i^z|0\rangle]$ is

$$m=\frac{1}{N}\sum_{\mu=1}^{N/3}\langle 0|(s^z_{1\mu}+s^z_{2\mu}+s^z_{3\mu})|0\rangle$$

$$=\frac{1}{N}\sum_{\mu=1}^{N/3}\langle' 0|T^\dagger(s^z_{1\mu}+s^z_{2\mu}+s^z_{3\mu})T|0'\rangle, \tag{A10}$$

where $|0'\rangle$ is the ground state in the renormalized Hilbert space ($T|0'\rangle=|0\rangle$). By using Eq. (A9), the magnetization is calculated to be

$$m=\frac{1}{3}m', \quad g<1,$$

$$m=\frac{-1}{3}+\frac{1}{3}m', \quad g>1, \tag{A11}$$

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 Eq. (A11) gives

$$m=0, \quad g<1.$$

$$m=-0.5, \quad g>1. \tag{A12}$$

Similarly, we can use the definition of staggered magnetization $[sm=(1/N)\,\Sigma_i^N\langle 0|(-1)^i s_i^z|0\rangle]$ and repeat the steps in calculating m; the staggered magnetization is obtained to be

$$sm=0.5, \quad g<1$$

$$sm=0, \quad g>1. \tag{A13}$$

These results confirm the Néel 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

$$H'_{N/3}(k',g')=T^\dagger H_N(k,g)T$$

$$=\begin{cases}\dfrac{k}{4}\left(\dfrac{-2N}{3}\right)+k\Sigma_i^{N/3}(s_i'^z s_{i+1}'^z+g s_i'^z), & g<1,\\[2ex] \dfrac{kN(1-4g)}{12}+k(g-1)\Sigma_i^{N/3}s_i'^z, & g>1.\end{cases} \tag{A14}$$

Therefore the ground state energy per site is calculated to be

$$e_0=\frac{E_0}{kN}=\begin{cases}\dfrac{1}{4}\left(-\dfrac{2}{3}\right)\left(1+\dfrac{1}{3}+\dfrac{1}{9}\cdots\right)=\dfrac{-1}{4}, & g<1,\\[2ex] \dfrac{1-4g}{12}-\dfrac{2(g-1)}{12}=\dfrac{1-2g}{4}, & g>1,\end{cases} \tag{A15}$$

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

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