New Universality Class in Spin-One-Half Fibonacci Heisenberg Chains

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Low energy properties of the $S = 1/2$ antiferromagnetic Heisenberg chains with Fibonacci exchange modulation are studied using the real space renormalization group method for strong exchange modulation. Using the analytical solution of the recursion equation, the true asymptotic behavoir is revealed, which was veiled by the finite size effect in the previous numerical works. It is found that the ground state of this model belongs to a new universality class with a logarithmically divergent dynamical exponent which is neither like Fibonacci XY chains nor like XY chains with relevant aperiodicity.

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The magnetism of quasiperiodic systems has been the subject of continual studies since the discovery of quasicrystals in 1984 [1]. This problem has been attracting renewed interest after the synthesis of magnetic quasicrystals with well-localized magnetic moments [2]. The artificial formation of one- and two-dimensional quasiperiodic structures is also coming into the scope of experimental physics [3,4] thanks to the recent progress of nanotechnology and surface engineering. Possibly motivated by this experimental progress, the theoretical investigation of the quantum magnetism in one- and two-dimensional quasiperiodic systems is started by many authors [5–10].

The $S = 1/2$ Fibonacci XY chain, which is mapped onto the free fermion chain, has been studied extensively by Kohmoto and co-workers [11] by means of the exact renormalization group method from the early days of quasicrystal physics. It is shown that the ground state of the XY chain with Fibonacci exchange modulation is critical with finite nonuniversal dynamical exponents. This approach was extended to include other types of aperiodicity and anisotropy [12]. It is clarified that the criticality of the Fibonacci XY chain emerges from the marginal nature of the Fibonacci and other precious mean aperiodicity in this model. For the relevant aperiodicity, more singular behavior with a divergent dynamical exponent is realized even for the XY chain [12].

On the other hand, the investigation of the $S = 1/2$ Fibonacci Heisenberg chains started only in the late 1990's. The ground state of the uniform $S = 1/2$ Heisenberg chain is exactly solved by the famous Bethe ansatz method [13] and is known to be in the Luttinger liquid state with conformal invariance. This implies that the dynamical exponent z is unity and the specific heat C and susceptibility χ behave as $C \sim T$ and $\chi \sim$ const at low temperatures. This exact solution is related to the transfer matrix of the two-dimensional classical eight vertex model which can be solved exactly [13]. On the quasiperiodic lattice also, some two-dimensional classical models are known to have exact solution [14]. However, the exact solution of the Fibonacci Heisenberg chain is not derived from these exactly solvable vertex models. Therefore we must resort to the renormalization group approach to clarify the reliable low energy asymptotic behavior. For weak Fibonacci modulation, Vidal and coworkers [7] have shown that the Fibonacci modulation is relevant on the basis of the weak modulation renormalization group calculation. The present author carried out the density-matrix renormalization group (DMRG) calculation and investigated the scaling properties of the low energy spectrum [5,6]. In the present work, we employ the real space renormalization group (RSRG) method [15], which is valid for the strong modulation, to elucidate the ground state properties of the $S = 1/2$ antiferromagnetic Fibonacci Heisenberg chains. Surprisingly, the finite size scaling formula, which fitted the DMRG data in Ref. [5] well, turned out to be the artifact of the finite size crossover effect. The true asymptotic behavior is first revealed by the exact solution of the recursion equation obtained in the present paper. It is also explained why the DMRG data are well fitted by the formula assumed in Ref. [5] within the appropriate range of the system size.

Our Hamiltonian is given by

$$\mathcal{H} = \sum_{i=1}^{N-1} J_{\alpha_i} \boldsymbol{S}_i \boldsymbol{S}_{i+1} \qquad (J_{\alpha_i} > 0,\ \alpha_i = A \text{ or } B), \quad (1)$$

where $\boldsymbol{S}_i$'s are the spin-1/2 operators. The exchange couplings J_{α_i} ($= J_A$ or J_B) follow the Fibonacci sequence generated by the substitution rule:

$$A \rightarrow AB, \qquad B \rightarrow A. \quad (2)$$

If one of the couplings J_A or J_B is much larger than the other, we can decimate the spins coupled via the stronger exchange coupling and calculate the effective interaction between the remaining spins by the perturbation method with respect to the weaker coupling [15]. This type of decimation scheme has been used to investigate the magnetization process of the Fibonacci Heisenberg chains [8].

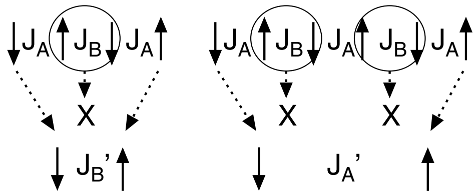

FIG. 1. The decimation procedure for $J_A \ll J_B$.

Here we apply this scheme to find the fixed point which governs the ground state in the absence of magnetization.

In the present work, we concentrate on the case of strong modulation, $\max(J_A/J_B, J_B/J_A) \gg 1$. For $J_A \ll J_B$, the spins connected by the J_B bonds are decimated as shown in Fig. 1. The spin-1/2 degrees of freedom survive on the sites in the middle of the sequence AA. The two kinds of sequences of bonds are allowed between two alive spins, namely, ABA and $ABABA$. Between these two alive spins, there exists one singlet pair in the former case while two singlet pairs exist in the latter case. Therefore the effective coupling is weaker for the latter case. This decimation process replaces the sequence $ABABA$ by A' and ABA sandwiched by two As by B' resulting in the sequence $B'A'B'A'A'B'A'B'A' \ldots$. Except for B' at the leftmost position, this sequence again gives the Fibonacci sequence as schematically shown in Fig. 2. As seen from the change of the number of the bonds by one step of decimation, this procedure essentially corresponds to a 3-step deflation. The rigorous proof will be reported in a separate paper [16].

In the case $J_A \gg J_B$, the decimation precesses are shown in Fig. 3. The three spins connected by successive A bonds form a doublet which can be described as a single spin with magnitude 1/2. The spins connected by the isolated J_A bonds are decimated. Therefore this decimation process again corresponds to the replacement $ABABA \rightarrow A'$ and $ABA \rightarrow B'$. In this case, the resulting sequence is the exact Fibonacci sequence. After the first decimation the A' bond becomes weaker than the B' bonds. Therefore the decimation rule for the case $J_A \ll J_B$ applies for the further decimation procedure.

The effective coupling can be calculated by the straightforward perturbation theory in weaker coupling. For the nth iteration, we have

$$J_A^{(n+1)} = \frac{J_A^{(n)3}}{4J_B^{(n)2}}, \qquad J_B^{(n+1)} = \frac{J_A^{(n)2}}{2J_B^{(n)}}, \tag{3}$$

with

$$J_A^{(1)} = \frac{J_A^3}{4J_B^2}, \qquad J_B^{(1)} = \frac{J_A^2}{2J_B}, \quad \text{for } J_B \gg J_A, \tag{4}$$

$$J_A^{(1)} = \frac{2J_B^2}{9J_A}, \qquad J_B^{(1)} = \frac{4J_B}{9}, \quad \text{for } J_A \gg J_B, \tag{5}$$

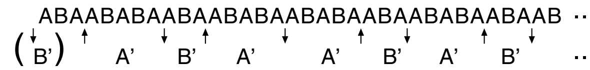

FIG. 2. The RSRG scheme of the Fibonacci Heisenberg chain. The letters A and B correspond to the bonds and the up and down arrows to the spins which survive decimation. For $J_A \gg J_B$ the leftmost spin and bond in the parentheses do not appear.

where the variables with $^{(n)}$ refer to the values after n-step iteration.

The ratio $J_A^{(n)}/J_B^{(n)}$ decreases under renormalization as

$$\frac{J_A^{(n+1)}}{J_B^{(n+1)}} = \frac{1}{2}\frac{J_A^{(n)}}{J_B^{(n)}} \qquad (n \geq 1). \tag{6}$$

This implies that the perturbation approximation becomes even more accurate as the renormalization proceeds. Therefore the aperiodicity is relevant in consistency with the result of the weak modulation renormalization group method [7]. Taking both results into account, we may safely expect that the ground state of the Fibonacci Heisenberg chain is governed by the strong modulation fixed point obtained in the present approach in the entire parameter range of $J_A/J_B \neq 1$.

The solution of the recursion equation (3) is given by

$$\begin{aligned} J_A^{(n)} &= J_A\left(\frac{J_A}{J_B}\right)^{2n} 2^{-n(n+1)}, \\ J_B^{(n)} &= J_B\left(\frac{J_A}{J_B}\right)^{2n} 2^{-n^2}, \quad \text{for } J_B \gg J_A, \end{aligned} \tag{7}$$

$$\begin{aligned} J_A^{(n)} &= \frac{8J_B}{9}\left(\frac{J_B}{J_A}\right)^{2n-1} 2^{-n(n+1)}, \\ J_B^{(n)} &= \frac{8J_A}{9}\left(\frac{J_B}{J_A}\right)^{2n-1} 2^{-n^2}, \quad \text{for } J_B \ll J_A. \end{aligned} \tag{8}$$

The length of the 3nth Fibonacci sequence is equal to the Fibonacci number F_{3n} which grows as ϕ^{3n} for large n where ϕ is the golden mean $[= (1 + \sqrt{5})/2]$. Therefore the chain of length $N \sim \phi^{3n}$ reduces to a single pair of spins after n decimation steps. This implies that the smallest energy scale ΔE for the finite Fibonacci chain with length N scales as

$$\begin{aligned} \Delta E \sim 2^{-n^2} &\sim \exp[-(\ln N/3\ln\phi)^2 \ln 2] \\ &= e^{-\kappa(\ln N)^2} = N^{-\kappa \ln N}, \\ &\text{with } \kappa \equiv \ln 2/(3\ln\phi)^2 \end{aligned} \tag{9}$$

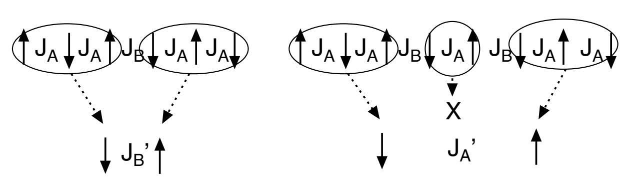

FIG. 3. The decimation procedure for $J_A \gg J_B$.

for large enough N, irrespective of the value of J_A/J_B. It should be noted that the dynamical exponent diverges logarithmically.

This size dependence implies that the number $ND(\Delta E)d\Delta E$ of the magnetic excited states with energies in the interval $\Delta E \sim \Delta E + d\Delta E$ scales as

$$\begin{aligned} ND(\Delta E)d\Delta E &\sim f\left[N\exp\left(-\sqrt{\frac{1}{\kappa}\ln\frac{1}{\Delta E}}\right)\right]d\left[N\exp\left(-\sqrt{\frac{1}{\kappa}\ln\frac{1}{\Delta E}}\right)\right] \\ &\sim Nf\left[N\exp\left(-\sqrt{\frac{1}{\kappa}\ln\frac{1}{\Delta E}}\right)\right]\frac{1}{2\kappa\Delta E\sqrt{\frac{1}{\kappa}\ln\frac{1}{\Delta E}}}\exp\left(-\sqrt{\frac{1}{\kappa}\ln\frac{1}{\Delta E}}\right)d\Delta E \end{aligned} \tag{10}$$

with a scaling function $f(x)$. Because the density of state per site $D(\Delta E)$ should be finite in the thermodynamic limit $N \to \infty$, the scaling function $f(x)$ tends to a finite value as $x \to \infty$. Therefore we find

$$D(\Delta E)d\Delta E \sim \frac{1}{2\kappa\Delta E\sqrt{\frac{1}{\kappa}\ln\frac{1}{\Delta E}}}\exp\left(-\sqrt{\frac{1}{\kappa}\ln\frac{1}{\Delta E}}\right)d\Delta E \tag{11}$$

for large enough N. Accordingly, the low temperature magnetic specific heat C should behave as

$$\begin{aligned} C &\sim \frac{\partial}{\partial T}N\int_0^T \Delta E D(\Delta E)d\Delta E \sim NTD(T) \\ &\sim \frac{N}{2\kappa\sqrt{\frac{1}{\kappa}\ln\frac{1}{T}}}\exp\left(-\sqrt{\frac{1}{\kappa}\ln\frac{1}{T}}\right). \end{aligned} \tag{12}$$

The magnetic susceptibility at temperature T should be the Curie contribution from the spins alive at the energy scale T. The number $n_s(T)$ of such spins is given by

$$n_s(T) \sim 2N\int_0^T D(\Delta E)d\Delta E, \tag{13}$$

because two spins are excited by breaking a single effective bond with effective exchange energy less than k_BT. Therefore the low temperature magnetic susceptibility χ behaves as

$$\chi(T) \sim \frac{2N}{4T}\int_0^T \frac{\exp(-\sqrt{\frac{1}{\kappa}\ln\frac{1}{\Delta E}})}{2\kappa\Delta E\sqrt{\frac{1}{\kappa}\ln\frac{1}{\Delta E}}}d\Delta E \sim \frac{N\exp(-\sqrt{\frac{1}{\kappa}\ln\frac{1}{T}})}{2T}. \tag{14}$$

This low temperature behavior should be contrasted with that of the uniform $S = 1/2$ antiferromagnetic Heisenberg chain $C \sim T$ and $\chi \sim$ const which is less singular than the present Fibonacci case. This is due to the logarithmic divergence of the dynamical exponent in the present case. To check the reliability of the present RSRG scheme, we also applied the same procedure for the Fibonacci XY chain to find

$$\Delta E \sim N^{-z} \tag{15}$$

with $z = (2/3\ln\phi)\ln\{\max[(J_A/J_B), (J_B/J_A)]\}$. This reproduces the exact result by Kohmoto and co-workers [11] in the limit $\max[(J_A/J_B), (J_B/J_A)] \gg 1$. Therefore our RSRG scheme is reliable at least for strong modulation.

The present results appear to be in contradiction with the results of Ref. [5], in which the present author carried out the DMRG calculation for the Fibonacci antiferromagnetic Heisenberg chains. In Ref. [5], we performed the finite size scaling analysis of the lowest energy gap ΔE based on the *assumption* that it will behave in the same way as the XY chain with relevant aperiodicity, namely, as $\Delta E \sim \exp(-cN^{\omega})$. However, the present analysis suggests a different behavior. Although we tried to replot the previous data using the scaling (9), the fit turned out to be very poor. The reason of this discrepancy will be understood in the following way.

For finite J_A/J_B, the perturbation approximation requires the higher order corrections which modify the recursion equation (3) in the form:

$$\begin{aligned} J_A^{(n+1)} &= \frac{J_A^{(n)3}}{J_B^{(n)2}}f_A(J_A^{(n)}/J_B^{(n)}), \\ J_B^{(n+1)} &= \frac{J_A^{(n)2}}{J_B^{(n)}}f_B(J_A^{(n)}/J_B^{(n)}). \end{aligned} \tag{16}$$

It should be noted that the correction factors f_A and f_B depend only on the ratio $J_A^{(n)}/J_B^{(n)}$ and satisfy $f_A(0) = 1/4$, $f_B(0) = 1/2$. This leads to the recursion equation for $\boldsymbol{X}^{(n)} = (X_A^{(n)}, X_B^{(n)}) \equiv (\ln J_A^{(n)}, \ln J_B^{(n)})$ as

$$\boldsymbol{X}^{(n+1)} = \begin{pmatrix} 3 & -2 \\ 2 & -1 \end{pmatrix}\boldsymbol{X}^{(n)} + \boldsymbol{\mu}(X_A^{(n)} - X_B^{(n)}) \tag{17}$$

with $\boldsymbol{\mu} = (\mu_A, \mu_B) \equiv (\ln f_A, \ln f_B)$. If the function $\boldsymbol{\mu}(X)$ is approximated by a linear function of X as $\boldsymbol{\mu}(X) = \boldsymbol{\gamma}X + \boldsymbol{\mu}_0$ with $\boldsymbol{\mu} = (\gamma_A, \gamma_B)$, we have

$$\boldsymbol{X}^{(n+1)} = M_m\boldsymbol{X}^{(n)} + \boldsymbol{\mu}_0, \tag{18}$$

where M_m is a 2×2 matrix

$$M_m = \begin{pmatrix} 3 - \gamma_A & -2 + \gamma_A \\ 2 - \gamma_B & -1 + \gamma_B \end{pmatrix}. \tag{19}$$

One of the eigenvalues of M_m is unity. If another eigenvalue $\lambda_m (\equiv 1 + \gamma_B - \gamma_A)$ is larger than unity, the solution of (18) grows with n as

$$X^{(n)} \propto \lambda_m^n. \tag{20}$$

In this case, both $\ln J_A^{(n)}$ and $\ln J_B^{(n)}$ scale as λ_m^n. Therefore the lowest energy scale of the chain of length N also scales as

$$\Delta E \sim \exp(-C\lambda_m^{[(\ln N)/(3\ln\phi)]}) \sim \exp(-CN^{[(\ln\lambda_m)/(3\ln\phi)]}) \sim \exp(-CN^{\omega}) \quad \text{with } \omega \equiv \frac{\ln\lambda_m}{3\ln\phi} \tag{21}$$

within appropriate range of system size N. This is the reason why the behavior (21) is observed in the DMRG calculation for finite systems. We have numerically diagonalized the Hamiltonian of the clusters $BAABABAAB$ and $BABAABAABAB$ which reduce to a single A' bond and B' bond after decimating B bonds. Using these numerical data, it is verified that the effective value of λ_m is larger than unity although it actually depends on J_A/J_B. As the renormalization proceeds, of course, the ratio J_A/J_B decreases and the true asymptotic behavior (9) is reached. More details of this calculation are presented in [16].

This crossover behavior implies that the extremely low temperature is required to observe the true asymptotic behavior (12) and (14) in weak modulation regime. Instead, the behaviors expected from (21), namely, $C \sim 1/(\ln T)^{1+1/\omega}$ and $\chi \sim 1/(T(\ln T)^{1/\omega})$ [12] would be observed in the intermediate temperature regime.

In summary, using the RSRG method, we have shown that the ground state of the $S = 1/2$ Fibonacci Heisenberg chain belongs to a new universality class in which the energy gap scales as $\exp(-\kappa(\ln N)^2)$ where κ is a universal constant independent of modulation strength. The low temperature behavior of the magnetic specific heat and magnetic susceptibility is predicted. The relationship to the previous numerical results [5] which appear to contradict the present calculation is also discussed. The details of the calculation and proof will be reported in a separate paper, which will also include the discussion of the general XXZ case [6] and ground state phase diagram [16].

We have found a new quantum dynamical critical behavior (9) which was so far unknown in the field of the quantum many body problem. Similar "singular dynamic scaling" is, however, known since the 1980's for the classical Ising model on the percolation clusters with Glauber dynamics [17]. In spite of the geometrical self-similarity common to this classical model and our quantum model, they look very different in many aspects. Although the underlying physics is still unclear, further investigation on this point might lead to a more profound understanding of both systems.

After this work was completed, the preprint by Vieira [18] appeared in the e-print archive in which some of the present results are derived. In addition, Vieira satisfactorily applied this method to the Heisenberg chains with relevant aperiodicity. A similar approach is also applied to the two-dimensional quasicrystal [10]. We thus expect the RSRG method is widely applicable to various problems in the field of quantum magnetism in quasiperiodic systems.

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