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Quantum phase transitions of periodic anisotropic XY chain in a transverse field

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Abstract

The transfer matrix method is used to study the quantum phase transitions of the uniform and periodic anisotropic XY quantum spin chain in a transverse field, which is defined by $H = -\frac{1}{2}\sum_n [J_n(\sigma_n^x\sigma_{n+1}^x + \alpha\sigma_n^y\sigma_{n+1}^y) + h\sigma_n^z]$. In zero temperature, it is found that the quantum phase transition point corresponds to $h/J = 1 + \alpha$, for uniform chain ($J_n = J$). For periodic chain, there is more than one phase transition point at some parameter region. In case the couplings take two alternating values, with ratio γ, the number of phase transition points are dependent on the parameters (α and γ) and the structure of the systems. These are different from that of quantum Ising chain in a transverse field. The critical points and the conditions of their existence are obtained analytically for period-two and three chains. The results are in good agreement with numerical results. The reasons of quantum phase transitions are discussed.

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1. Introduction

The zero temperature quantum critical phenomena and low temperature thermodynamical behaviors of quantum spin chains have been a subject of very active research over several decades [1–3]. Among the most frequently studied quantum spin chains, the quantum Ising chain [3] in a transverse field and quantum XY chain [2] are the simplest models. The physical properties of quantum Ising and XY chains can be studied by the famous Jordan–Wigner transformation [2,3], which transfers the spin operator to spinless Fermi operator in the quadratic form and can be diagonalized analytically. The quantum critical phenomena of the random quantum Ising and XY chains are studied by renormalization-group method [4] and numerical method [5]. Recently, the quantum phase transition of the quasiperiodic quantum Ising [6–8] and XY chains [9,10] have been extensively studied by the transfer matrix method and numerical method. The quantum critical points are found for different kinds of quasiperiodic and aperiodic chains and the

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universality class of the chains are determined by the fluctuation of the sums of any number of consecutive couplings of the chains at the critical points [8]. Also, the quantum Ising [11] and XY [12] chains are used to test the density matrix renormalization group method proposed by White [13,14].

Another interesting quantum spin model is the anisotropic XY chain in a transverse field [15–22], which makes QI and XY chains as special cases and was used to study the crossover from Ising to isotropic XY behaviors. Perk et al. [17] discussed the thermodynamical properties of periodic isotropy XY chain in a transverse field with Dzyaloshinskii–Moriya interaction. Satija and Chaves [23] studied the excitation spectra of quasiperiodic anisotropic XY chains at some special parameter values and crossover from Ising to XY behaviors. Recently, Derzhko et al. have studied the thermodynamical behaviors of periodic nonuniform and random quantum XY chain in a transverse field [19–22]. But study on the relationship between the thermodynamical and ground state behaviors is still lacking. It is well known [24] that the properties of periodic spin systems can provide insight into the random spin system. Therefore, the study on the properties of ground state, such as quantum phase transitions, of periodic anisotropic XY chain in a transverse field is useful for the understanding of thermodynamical and dynamical behavior of periodic nonuniform and random systems. However, to our knowledge, there is no such study up to now.

On the other hand, there are three ingredients in the periodic anisotropic XY chain in a transverse field. These are the ratio γ of two kinds of exchange interaction, anisotropic parameter α and ratio h of external field to exchange interaction. This is different from that of QI, which has two ingredients (γ and h). Therefore, if the periodic anisotropic XY chain can exhibit new phenomena that is also an interesting problem. In this paper, our aim was to study the ground state properties of this model. The paper is organized as following. In Section 2, we give the model and calculating methods. The analytical and numerical results of uniform and periodic models are given in Sections 3 and 4. In Section 5, we present discussion on the reasons for the quantum phase transitions and some conclusions.

2. Model and formula

The anisotropic XY quantum chain spin in a transverse field is defined by the following Hamiltonian:

$$H = -\frac{1}{2}\sum_{n}[J_n(\sigma_n^x\sigma_{n+1}^x + \alpha\sigma_n^y\sigma_{n+1}^y) + h\sigma_n^z]. \tag{1}$$

Here, $\sigma^{x,y,z}$ are the Pauli matrices, J_n are the nearest neighbor interactions, h is a uniform external transverse field and $0<\alpha<1$ is a parameter characterizing the degree of anisotropy of the interactions in the xy plane. The quantum Ising chain in a transverse field and anisotropic XY chain correspond to $\alpha = 0$ and $h = 0$, respectively. By using the Jordan–Wigner transformation [2], the Hamiltonian (1) can be written by spinless fermion operator, which yields

$$H = \sum_{n,m}[c_n^\dagger A_{nm}c_m + \tfrac{1}{2}(c_n^\dagger B_{nm}c_m^\dagger + \text{h.c.})], \tag{2}$$

where c_n and $c_n^\dagger$ are the anticommuting fermion operators. In Eq. (2), we neglect the constant and boundary terms. For the chain with N spins and periodic boundary condition, the two $N \times N$ matrices $\mathbf{A}$ and $\mathbf{B}$ are

$$\mathbf{A} = \begin{pmatrix} -h_1 & -\frac{1}{2}J_1(1+\alpha) & 0 & \cdots & -\frac{1}{2}J_N(1+\alpha) \\ -\frac{1}{2}J_1(1+\alpha) & -h_2 & -\frac{1}{2}J_2(1+\alpha) & \cdots & 0 \\ 0 & -\frac{1}{2}J_2(1+\alpha) & -h_3 & \cdots & 0 \\ . & . & . & \cdots & . \\ -\frac{1}{2}J_N(1+\alpha) & 0 & 0 & \cdots & -h_N \end{pmatrix} \tag{3}$$

and

$$\mathbf{B}=\begin{pmatrix} 0 & -\frac{1}{2}J_1(1-\alpha) & 0 & \cdots & \frac{1}{2}J_N(1-\alpha) \\ \frac{1}{2}J_1(1-\alpha) & 0 & -\frac{1}{2}J_2(1-\alpha) & \cdots & 0 \\ 0 & \frac{1}{2}J_2(1-\alpha) & 0 & \cdots & 0 \\ . & . & . & \cdots & . \\ -\frac{1}{2}J_N(1-\alpha) & 0 & 0 & \cdots & 0 \end{pmatrix}, \tag{4}$$

respectively.

Eq. (2) can be diagonalized by following the Bogoliubov transformation

$$\eta_k=\tfrac{1}{2}\sum_n[(\phi_{k,n}+\psi_{k,n})c_n+(\phi_{k,n}-\psi_{k,n})c_n^+],$$
$$\eta_k^+=\tfrac{1}{2}\sum_n x[(\phi_{k,n}+\psi_{k,n})c_n^+ +(\phi_{k,n}-\psi_{k,n})c_n]. \tag{5}$$

The Hamiltonian of the spin chain thus takes the following form:

$$H=\sum_{k=1}^{N}\Lambda_k(\eta_k^+\eta_k-\tfrac{1}{2}). \tag{6}$$

The excitation energies $\Lambda_k>0$ and the coefficients $\{\phi_{k,n},\psi_{k,n}\}$ of the Bogoliubov transformation (5) are the generalized eigenvalues and eigenvectors of the following equations:

$$\Lambda_k\psi_{k,n}=-J_{n-1}\phi_{k,n-1}-h\phi_{k,n}-\alpha J_n\phi_{k,n+1},$$
$$\Lambda_k\phi_{k,n}=-\alpha J_{n-1}\psi_{k,n-1}-h\psi_{k,n}-J_n\psi_{k,n+1}. \tag{7}$$

Eq. (7) is equivalent to the following next nearest neighbor tight-binding equation:

$$\Lambda^2\psi_n=\alpha J_{n-1}J_{n-2}\psi_{n-2}+J_{n-1}h(1+\alpha)\psi_{n-1}+(h^2+J_{n-1}^2+\alpha^2J_n^2)\psi_n$$
$$+J_nh(1+\alpha)\psi_{n+1}+\alpha J_{n+1}J_n\psi_{n+2}. \tag{8}$$

Here we omit the subscripts k of Λ_k and $\psi_{k,n}$ for simplicity of the expressions.

Also, the Λ^2 are the solutions of equation

$$\det[(\mathbf{A}-\mathbf{B})(\mathbf{A}+\mathbf{B})-\Lambda^2\mathbf{I}]=0, \tag{9}$$

where $\mathbf{I}$ is the unit matrix of $N\times N$.

Eq. (8) can be rewritten in following transfer matrix form:

$$\mathbf{\Psi}_n\equiv\begin{pmatrix}\psi_{n+2}\\ \psi_{n+1}\\ \psi_n\\ \psi_{n-1}\end{pmatrix}=\begin{pmatrix} -\frac{J_nh(1+\alpha)}{\alpha J_{n+1}J_n} & \frac{\Lambda^2-h^2-J_{n-1}^2-\alpha^2J_n^2}{\alpha J_{n+1}J_n} & -\frac{J_{n-1}h(1+\alpha)}{\alpha J_{n+1}J_n} & -\frac{J_{n-1}J_{n-2}}{J_{n+1}J_n} \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}\begin{pmatrix}\psi_{n+1}\\ \psi_n\\ \psi_{n-1}\\ \psi_{n-2}\end{pmatrix}$$
$$\equiv\mathbf{M}_n(\Lambda^2)\mathbf{\Psi}_{n-1}. \tag{10}$$

Therefore, $\mathbf{\Psi}_N=\mathbf{M}^{(N)}(\Lambda^2)\mathbf{\Psi}_0$ with $\mathbf{M}^{(N)}(\Lambda^2)\equiv\mathbf{M}_N(\Lambda^2)\mathbf{M}_{N-1}\cdots\mathbf{M}_1(\Lambda^2)$.

In zero temperature, the quantum critical points correspond to parameter values that satisfy the condition $\Lambda=0$. Following Eq. (9), we can see that $\det[(\mathbf{A}-\mathbf{B})(\mathbf{A}+\mathbf{B})]=0$ at $\Lambda=0$. Because of $(\mathbf{A}+\mathbf{B})=(\mathbf{A}-\mathbf{B})^{\mathrm{T}}$, it reduces $\det(\mathbf{A}-\mathbf{B})=0$. This equation gives the relation of parameter values at quantum critical points and was used to study the quantum critical points for random [25] and quasiperiodic quantum Ising chains [6–8]. But this method is very complicated in our case because of Eq. (8) involving the next nearest neighbor terms. The quantum critical points also correspond to the

parameter values, making the modules of the four eigenvalues of matrix $\mathbf{M}^{(N)}$ equal one. We will use this method to find the critical values for uniform and periodic quantum chains.

3. Analytical results

3.1. Uniform case

For the uniform quantum spin chain, $J_n = J$, Eq. (8) becomes

$$\Lambda^2\psi_n = \alpha J^2\psi_{n-2} + Jh(1+\alpha)\psi_{n-1} + [h^2 + (1+\alpha^2)J^2]\psi_n + Jh(1+\alpha)\psi_{n+1} + \alpha J^2\psi_{n+2}. \tag{11}$$

The transfer matrix $\mathbf{M}^{(N)}(\Lambda = 0) = \mathbf{M}^N$ with

$$\mathbf{M} = \begin{pmatrix} -\frac{x(1+\alpha)}{\alpha} & -\frac{x^2+(1+\alpha^2)}{\alpha} & -\frac{x(1+\alpha)}{\alpha} & -1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix} \tag{12}$$

and $x = h/J$.

The condition of the unimodularity of the eigenvalue of $\mathbf{M}^{(N)}$ corresponds to $|\lambda_r| = 1$ with λ_r $(r = 1, 2, 3, 4)$ being four eigenvalues of $\mathbf{M}$. The eigenvalue equation of $\mathbf{M}$ is

$$\lambda^4 + b\lambda^3 + c\lambda^2 + b\lambda + 1 = 0 \tag{13}$$

with

$$b = \frac{x(1+\alpha)}{\alpha} \quad \text{and} \quad c = \frac{x^2 + (1+\alpha^2)}{\alpha}, \tag{14}$$

respectively.

The solutions of Eq. (13) are

$$\lambda_{1,2,3,4} = \frac{y_\pm \pm \sqrt{y_\pm^2 - 4}}{2}, \qquad y_\pm = \frac{-b \pm \sqrt{b^2 - 4c + 8}}{2}, \tag{15}$$

then the condition of $|\lambda_r| = 1$ gives $y = \pm 2$. That is

$$2 + c = -2b \quad \text{or} \quad 2 + c = 2b. \tag{16}$$

The first equation has no solution for $\alpha, J, h > 0$. The solution of second equation is

$$x_c = \left(\frac{h}{J}\right)_c = 1 + \alpha. \tag{17}$$

Now we check condition (17) by solving Eq. (11) directly. Because of the uniformity, we can assume the solution of Eq. (11) is $\psi_n = Ce^{ink}$. Substituting into Eq. (11), we obtain

$$\Lambda^2 = J^2[2\alpha\cos(2k) + 2(1+\alpha)x\cos(k) + x^2 + (1+\alpha^2)]. \tag{18}$$

The Λ^2 has minimal value at $\sin k = 0$ for $x > x_1$ and minimal value at $\cos k = -x(1+\alpha)/4\alpha$ for $x \leqslant x_1$ with $x_1 = 4\alpha/(1+\alpha)$. The minimal value of Λ^2 is

$$\Lambda^2_{\min} = \begin{cases} [(1+\alpha) - x]^2 J^2 & \text{for } x > x_1, \\ \dfrac{(1-\alpha)^2(2\sqrt{\alpha} - x)(2\sqrt{\alpha} + x)}{4\alpha} J^2 & \text{for } x \leqslant x_1. \end{cases} \tag{19}$$

From Eq. (19), we can see that $\Lambda^2_{\min}$ is always large than zero for $x \leqslant x_1$. For $x > x_1$, the critical parameter value of $\Lambda^2_{\min} = 0$ is $x = x_c = 1 + \alpha$, which is large than x_1. Therefore, the quantum critical point of uniform spin chain corresponds to $x = x_c$.

3.2. Period-two case

For the periodic quantum spin chain with $J_{2n} = J$ and $J_{2n+1} = \gamma J$, Eq. (8) can be rewritten as

$$\begin{aligned}
\Lambda^2\psi_{2n} &= \alpha\gamma J^2\psi_{2n-2} + (1+\alpha)\gamma Jh\psi_{2n-1} + [h^2 + J^2(\alpha^2+\gamma^2)]\psi_{2n} + (1+\alpha)Jh\psi_{2n+1} + \alpha\gamma J^2\psi_{2n+2},\\
\Lambda^2\psi_{2n+1} &= \alpha\gamma J^2\psi_{2n-1} + (1+\alpha)Jh\psi_{2n} + [h^2 + J^2(1+\alpha^2\gamma^2)]\psi_{2n+1} + (1+\alpha)\gamma Jh\psi_{2n+2} + \alpha\gamma J^2\psi_{2n+3}.
\end{aligned} \tag{20}$$

The transfer matrix $\mathbf{M}^{(N)}(\Lambda = 0) = \mathbf{T}^{N/2}$ with

$$\begin{aligned}
\mathbf{T} &= \begin{pmatrix} -\frac{(1+\alpha)x}{\alpha} & -\frac{x^2+(1+\alpha^2\gamma^2)}{\gamma\alpha} & -\frac{(1+\alpha)x}{\gamma\alpha} & -1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}\begin{pmatrix} -\frac{(1+\alpha)x}{\gamma\alpha} & -\frac{x^2+(\alpha^2+\gamma^2)}{\gamma\alpha} & -\frac{(1+\alpha)x}{\alpha} & -1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}\\
&= \begin{pmatrix} \frac{(1+\alpha)^2x^2}{\gamma\alpha^2} - \frac{x^2+(1+\alpha^2\gamma^2)}{\gamma\alpha} & \frac{(1+\alpha)x[x^2+(\alpha^2+\gamma^2)]}{\gamma\alpha^2} - \frac{(1+\alpha)x}{\gamma\alpha} & \frac{(1+\alpha)^2x^2}{\alpha^2} - 1 & \frac{(1+\alpha)x}{\alpha} \\ -\frac{(1+\alpha)x}{\gamma\alpha} & -\frac{x^2+(\alpha^2+\gamma^2)}{\gamma\alpha} & -\frac{(1+\alpha)x}{\alpha} & -1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}.
\end{aligned} \tag{21}$$

The eigenvalues $\lambda_{1,2,3,4}$ of matrix $\mathbf{T}$ satisfy Eq. (13) with

$$b = \frac{\alpha(1+\alpha^2)(1+\gamma^2) - (1+\alpha^2)x^2}{\gamma\alpha^2} \tag{22}$$

and

$$c = \frac{x^4 - 2\alpha x^2(1+\gamma^2) + (\alpha^2+\gamma^2+\alpha^4\gamma^2+\alpha^2\gamma^4+2\alpha^2\gamma^2)}{\gamma^2\alpha^2}. \tag{23}$$

As in the uniform case, the conditions $|\lambda_{1,2,3,4}| = 1$ satisfy Eq. (16). We obtain

$$\begin{aligned}
x_{c_1} &= \left(\frac{h}{J}\right)_{c_1} = \sqrt{(\alpha+\gamma)(1+\alpha\gamma)} \quad \text{for } 0<\alpha,\ \gamma<1,\\
x_{c_2} &= \left(\frac{h}{J}\right)_{c_2} = \sqrt{(\alpha-\gamma)(1-\alpha\gamma)} \quad \text{for } \alpha>\gamma
\end{aligned} \tag{24}$$

from the two equations (16), respectively.

Similarly, we can obtain Eqs. (24) by solving Eqs. (20) directly. Let $\psi_{2n} = Ce^{i2nk}$ and $\psi_{2n+1} = De^{i(2n+1)k}$, we obtain from Eqs. (20)

$$\begin{cases} [2\alpha\gamma J^2\cos(2k) + h^2 + J^2(\alpha^2+\gamma^2) - \Lambda^2]C + (1+\alpha)Jh(\gamma e^{-ik} + e^{ik})D = 0,\\ (1+\alpha)Jh(e^{-ik} + \gamma e^{ik})C + [2\alpha\gamma J^2\cos(2k) + h^2 + J^2(1+\alpha^2\gamma^2) - \Lambda^2]D = 0. \end{cases} \tag{25}$$

The nontrivial solutions of Eq. (25) satisfy

$$\begin{vmatrix} 2\alpha\gamma J^2\cos(2k) + h^2 + J^2(\alpha^2+\gamma^2) - \Lambda^2 & (1+\alpha)Jh(\gamma e^{-ik} + e^{ik}) \\ (1+\alpha)Jh(e^{-ik} + \gamma e^{ik}) & 2\alpha\gamma J^2\cos(2k) + h^2 + J^2(1+\alpha^2\gamma^2) - \Lambda^2 \end{vmatrix} = 0. \tag{26}$$

That is

$$\Lambda^4 - A\Lambda^2 + B = 0. \tag{27}$$

Here

$$A = J^2[4\alpha\gamma\cos(2k) + 2x^2 + (1+\alpha^2)(1+\gamma^2)] \tag{28}$$

and

$$\begin{aligned} B = J^4\{&[2\alpha\gamma\cos(2k) + x^2]^2 + [2\alpha\gamma\cos(2k) + x^2](1+\alpha^2)(1+\gamma^2) \\ &+ (\alpha^2+\gamma^2)(1+\alpha^2\gamma^2) - (1+\alpha)^2(2\gamma\cos(2k) + 1 + \gamma^2)x^2\}. \end{aligned} \tag{29}$$

The solutions of Eq. (27) are

$$\Lambda_{\pm}^2 = \tfrac{1}{2}(A \pm \sqrt{A^2 - 4B}). \tag{30}$$

In order to find solutions of $\Lambda^2 = 0$, we need to consider Λ_-^2 only. The minimal points of Λ_-^2 are

$$\begin{aligned} &\sin(2k) = 0, \quad \cos(2k) = 1 \quad \text{for } x > x_1, \\ &\cos(2k) = \tfrac{1}{2\gamma}\left[\frac{(1+\alpha)^2x^4 - \alpha^2(1-\alpha)^2(1-\gamma^2)^2}{4\alpha^2x^2} - 1 - \gamma^2\right] \quad \text{for } x_1 > x > x_2, \\ &\sin(2k) = 0, \quad \cos(2k) = -1 \quad \text{for } x < x_2. \end{aligned} \tag{31}$$

Here

$$x_1^2 = \frac{\alpha(1-\alpha)^2(1-\gamma)^2(1+\gamma)}{\sqrt{4\alpha^2(1+\gamma)^2 + (1-\alpha^2)^2(1-\gamma)^2} - 2\alpha(1+\gamma)} \tag{32}$$

and

$$x_2^2 = \frac{\alpha(1-\alpha)^2(1+\gamma)^2(1-\gamma)}{\sqrt{4\alpha^2(1-\gamma)^2 + (1-\alpha^2)^2(1+\gamma)^2} - 2\alpha(1-\gamma)}. \tag{33}$$

After a long calculation, we obtain

$$\Lambda_{\min}^2 = \begin{cases} \dfrac{2[(1+\alpha\gamma)(\gamma+\alpha) - x^2]^2}{A_1 + \sqrt{A_1^2 - 4B_1}}J^4 & \text{for } x > x_1, \\ \dfrac{(1-\alpha)^2[x^2 - \alpha(1-\gamma)^2][\alpha(1+\gamma)^2 - x^2]}{4\alpha x^2}J^2 & \text{for } x_1 > x > x_2, \\ \dfrac{2[(1-\alpha\gamma)(\alpha-\gamma) - x^2]^2}{A_2 + \sqrt{A_2^2 - 4B_2}}J^4 & \text{for } x < x_2 \end{cases} \tag{34}$$

with

$$A_{1,2} = J^2[2x^2 + (1+\alpha^2)(1+\gamma^2) \pm 4\alpha\gamma] \tag{35}$$

and

$$B_{1,2} = J^4\{[x^2 \pm 2\alpha\gamma]^2 + [x^2 \pm 2\alpha\gamma](1+\alpha^2)(1+\gamma^2) + (\alpha^2+\gamma^2)(1+\alpha^2\gamma^2) - (1+\alpha)^2(1\pm\gamma)^2x^2\}, \tag{36}$$

respectively.

It can be proven that $\Lambda_{\min}^2 > 0$ for $x_1 > x > x_2$. Therefore, the critical values corresponding to $\Lambda^2 = 0$ are $x_{c_1} = (h/J)_{c_1} = \sqrt{(\alpha+\gamma)(1+\alpha\gamma)} > x_1$ for any $0 < \alpha, \gamma < 1$ and $x_{c_2} = (h/J)_{c_2} = \sqrt{(\alpha-\gamma)(1-\alpha\gamma)} < x_2$ for $\alpha > \gamma$. That is, there is one critical point for $0 < \alpha < \gamma$ and two critical points for $\gamma < \alpha < 1$.

3.3. Period-three cases

For the period-three quantum spin chain with $J_{3n} = J_{3n+1} = J$, $J_{3n+2} = \gamma J$, Eq. (8) can be rewritten as

$$\begin{aligned}
\Lambda^2\psi_{3n} &= \alpha\gamma J^2\psi_{3n-2} + (1+\alpha)\gamma Jh\psi_{3n-1} + [h^2 + J^2(\alpha^2+\gamma^2)]\psi_{3n} + (1+\alpha)Jh\psi_{3n+1} + \alpha J^2\psi_{3n+2},\\
\Lambda^2\psi_{3n+1} &= \alpha\gamma J^2\psi_{3n-1} + (1+\alpha)Jh\psi_{3n} + [h^2 + J^2(1+\alpha^2)]\psi_{3n+1} + (1+\alpha)Jh\psi_{3n+2} + \alpha\gamma J^2\psi_{3n+3},\\
\Lambda^2\psi_{3n+2} &= \alpha J^2\psi_{3n} + (1+\alpha)Jh\psi_{3n+1} + [h^2 + J^2(1+\alpha^2\gamma^2)]\psi_{3n+2} + (1+\alpha)\gamma Jh\psi_{3n+3} + \alpha\gamma J^2\psi_{3n+4}. \qquad (37)
\end{aligned}$$

We use the transfer matrix method to determine the quantum critical points of systems. The transfer matrix $\mathbf{M}^{(N)}(\Lambda = 0) = \mathbf{T}^{N/3}$ with

$$\mathbf{T} = \begin{pmatrix} -\frac{(1+\alpha)x}{\alpha} & -\frac{x^2+\alpha^2\gamma^2+1}{\gamma\alpha} & -\frac{(1+\alpha)x}{\gamma\alpha} & -\frac{1}{\gamma} \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} -\frac{(1+\alpha)x}{\alpha\gamma} & -\frac{x^2+\alpha^2+1}{\gamma\alpha} & -\frac{(1+\alpha)x}{\gamma\alpha} & -1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$
$$\begin{pmatrix} -\frac{(1+\alpha)x}{\alpha} & -\frac{x^2+\alpha^2+\gamma^2}{\alpha} & -\frac{(1+\alpha)\gamma x}{\alpha} & -\gamma \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix} = \begin{pmatrix} T_{11} & T_{12} & T_{13} & T_{14} \\ T_{21} & T_{22} & T_{23} & T_{24} \\ T_{31} & T_{32} & T_{33} & T_{34} \\ T_{41} & T_{42} & T_{43} & T_{44} \end{pmatrix} \qquad (38)$$

with

$$\begin{aligned}
T_{11} &= \frac{(1+\alpha)x(2x^2+2+\alpha^2+\alpha^2\gamma^2)}{\gamma\alpha^2} - \frac{(1+\alpha)^3x^3}{\gamma\alpha^3} - \frac{(1+\alpha)x}{\gamma\alpha},\\
T_{12} &= \frac{(x^2+1+\alpha^2\gamma^2)(x^2+\alpha^2+\gamma^2)}{\gamma\alpha^2} - \frac{1}{\gamma} + \frac{(1+\alpha)^2x^2}{\gamma\alpha^2} - \frac{(1+\alpha)^2x^2(x^2+\alpha^2+\gamma^2)}{\gamma\alpha^3},\\
T_{13} &= \frac{(1+\alpha)x(x^2+1+\alpha^2\gamma^2)}{\alpha^2} - \frac{(1+\alpha)^3x^3}{\alpha^3} + \frac{(1+\alpha)x}{\alpha},\\
T_{14} &= \frac{x^2+1+\alpha^2\gamma^2}{\alpha} - \frac{(1+\alpha)^2x^2}{\alpha^2},\\
T_{21} &= \frac{(1+\alpha)^2x^2}{\alpha^2\gamma} - \frac{x^2+1+\alpha^2}{\alpha\gamma},\\
T_{22} &= \frac{(1+\alpha)x(x^2+\alpha^2+\gamma^2)}{\gamma\alpha^2} - \frac{(1+\alpha)x}{\alpha\gamma},\\
T_{23} &= \frac{(1+\alpha)^2x^2}{\alpha^2} - 1, \qquad T_{24} = \frac{(1+\alpha)x}{\alpha},\\
T_{31} &= -\frac{(1+\alpha)x}{\alpha}, \qquad T_{32} = -\frac{x^2+\gamma^2+\alpha^2}{\alpha},\\
T_{33} &= -\frac{\gamma(1+\alpha)x}{\alpha}, \qquad T_{34} = -\gamma\\
T_{41} &= 1, \qquad T_{42} = T_{43} = T_{44} = 0. \qquad (39)
\end{aligned}$$

The eigenvalues $\lambda_{1,2,3,4}$ of matrix $\mathbf{T}$ satisfy Eq. (13) with

$$b = \frac{1}{\alpha^3\gamma^2}(\gamma x^3 + \alpha^3\gamma x^3 - 2\alpha\gamma x - \alpha^4\gamma^3 x - \alpha\gamma^3 x - 2\alpha^4\gamma x) \qquad (40)$$

and

$$c = \frac{1}{\alpha^3\gamma^2}(x^6 - 4\alpha x^4 - 2\alpha\gamma^2 x^4 + 4\alpha^2\gamma^2 x^2 + \alpha^2\gamma^4 x^2 + 4\alpha^2 x^2 + \alpha^6\gamma^2 + \gamma^2). \tag{41}$$

Same as in the uniform case, the conditions $|\lambda_{1,2,3,4}| = 1$ give Eq. (16). Now, the two equations of Eqs. (16) become

$$x(x^2 - 2\alpha - \alpha\gamma^2) + \gamma(1 + \alpha^3) = 0 \tag{42}$$

and

$$x(x^2 - 2\alpha - \alpha\gamma^2) - \gamma(1 + \alpha^3) = 0. \tag{43}$$

Eqs. (42) and (43) have only real root for $\alpha < \alpha_c(\gamma)$ and three real roots for $1 > \alpha > \alpha_c(\gamma)$ with $\alpha_c(\gamma)$ is only real root of

$$\alpha_c^3(\gamma) = \frac{2(2+\gamma^2)^3 - 27\gamma^2 - 2\sqrt{(2+\gamma^2)^3[(2+\gamma^2)^3 - 27\gamma^2]}}{27\gamma^2}. \tag{44}$$

In Table 1, we give some values of α_c as a function of γ.

For $0 < \alpha < \alpha_c(\gamma)$, the only real root x of Eq. (43) is

$$x = \sqrt{-\frac{q}{2} + \sqrt{\Delta}3} + \sqrt{-\frac{q}{2} - \sqrt{\Delta}3} > 0. \tag{45}$$

Here $\Delta = (q/2)^2 + (p/3)^3$ and $q = \gamma(1 + \alpha^3)$, $p = -\alpha(2 + \gamma^2)$. And the real root of Eq. (42) is $-x < 0$.

For $\alpha_c(\gamma) < \alpha < 1$, let $x_{1,2,3}$ ($y_{1,2,3}$) are three roots of Eq. (42) (Eq. (43)). Then

$$\begin{aligned} x_1 &= -y_2 = 23\sqrt{r}\cos\theta > 0, \\ x_2 &= -y_1 = 23\sqrt{r}\cos\left(\theta + \frac{2\pi}{3}\right) < 0, \\ x_3 &= -y_3 = 23\sqrt{r}\cos\left(\theta + \frac{4\pi}{3}\right) > 0 \end{aligned} \tag{46}$$

with $r = \sqrt{-(p/3)^3}$ and $\theta = (1/3)\arccos(-q/2r)$. Three quantum phase transition points correspond to $x_{c_1} = x_3$, $x_{c_2} = x_1$ and $x_{c_3} = y_1$, respectively. In Table 2, we give the three x_c for $\alpha_c(\gamma) < \alpha < 1$ with $\gamma = 0.5$. Therefore, there is one quantum critical point for $0 < \alpha < \alpha_c(\gamma)$ and three critical points for $\alpha_c(\gamma) < \alpha < 1$, respectively.

Table 1
The α_c of the period-three chain for different γ

γ	α_c
0.10	0.2037084603266
0.20	0.3239706080471
0.30	0.4258317020335
0.40	0.5180601963376
0.50	0.6044018928382
0.60	0.6869330838122
0.70	0.7669701609132
0.80	0.8454178497614
0.90	0.9229309755193
1.00	0.9999999949418

Table 2
The three critical values of the period-three chain for different $1 > \alpha > \alpha_c(\gamma)$. The $\gamma = 0.5$ and $\alpha_c = 0.6044018928382$

α	x_{c_1}	x_{c_2}	x_{c_3}
0.65	0.5487657865523	0.8376612082019	1.3864269947543
0.70	0.5111362486349	0.9187635160204	1.4298997646553
0.75	0.4917743315936	0.9813530328152	1.4731273644088
0.80	0.4823448144253	1.0337815566612	1.5161263710866
0.85	0.4797171990038	1.0791954390936	1.5589126380973
0.90	0.4823240292046	1.1191771519804	1.6015011811850
0.95	0.4892677729025	1.1546383475330	1.6439061204355
1.00	0.4999999999999	1.1861406616346	1.6861406616345

4. Numerical results

Now, we turn to study the order parameters $M_{x,y,z} = \langle \mathrm{GS}|\sigma^{x,y,z}|\mathrm{GS}\rangle|\mathrm{GS}\rangle$ being the ground state of spin chain. However, even in the ordered state, the order parameters $M_{x,y} = \langle \mathrm{GS}|\sigma^{x,y}|\mathrm{GS}\rangle$ cannot be obtained due to the invariance of the Hamiltonian when σ_n^x (σ_n^y) is changed to $-\sigma_n^x$ ($-\sigma_n^y$). On the contrary, the $M_z = \langle \mathrm{GS}|\sigma^z|\mathrm{GS}\rangle$ and the correlation functions $C_l^{x,y} = \langle \mathrm{GS}|\sigma_1^{x,y}\sigma_{1+l}^{x,y}|\mathrm{GS}\rangle$ can be obtained. Same as that of Ref. [6], we use the long range correlation function C_L^x (L is half of the length of spin chain) and M_z as the order parameters.

Following the method used by Lieb et al. [2], we get the following results:

$$C_L^x = \begin{vmatrix} G_{1,2} & G_{1,3} & \cdots & G_{1,L+1} \\ \vdots & \vdots & \vdots & \vdots \\ G_{L,2} & G_{L,3} & \cdots & G_{L,L+1} \end{vmatrix} \tag{47}$$

and

$$M_z = -\frac{1}{N}\sum_n G_{n,n} \tag{48}$$

with

$$G_{i,j} = -\sum_k \psi_{k,i}\phi_{k,j}. \tag{49}$$

Here $\psi_{k,i}$ and$\phi_{k,i}$ are eigenfunctions of Eq. (7).

The numerical results are shown in Figs. 1 and 2 for uniform and period-two chains, respectively. The results are obtained by finding the eigenvalues and eigenvectors of matrix $(\mathbf{A}+\mathbf{B})(\mathbf{A}-\mathbf{B})$ for finite length spin chain with periodic boundary condition numerically. In Fig. 1, we plot C_L^x and M_z of uniform chain with 100 spins as functions of $x = h/J$ for different α, respectively. The results obtained from a longer chain are almost the same. From Fig. 1, we can see that it undergoes a phase transition at the critical value where the correlation function C_L^x vanishes and the M_z is nonanalytic. The numerical results for the critical value fits the analytical result (17) very well.

In Fig. 2, we plot C_L^x and M_z of the period-two chain with 128 spins as functions of $x = h/J$ for different α, respectively. The results obtained from a longer chain are almost the same. From Fig. 2, we can see that it undergoes a phase transition at the critical value for $\alpha \leqslant \gamma$ and two phase transitions for $\alpha > \gamma$. Also, the numerical results for the critical values fit analytical results (24) very well.

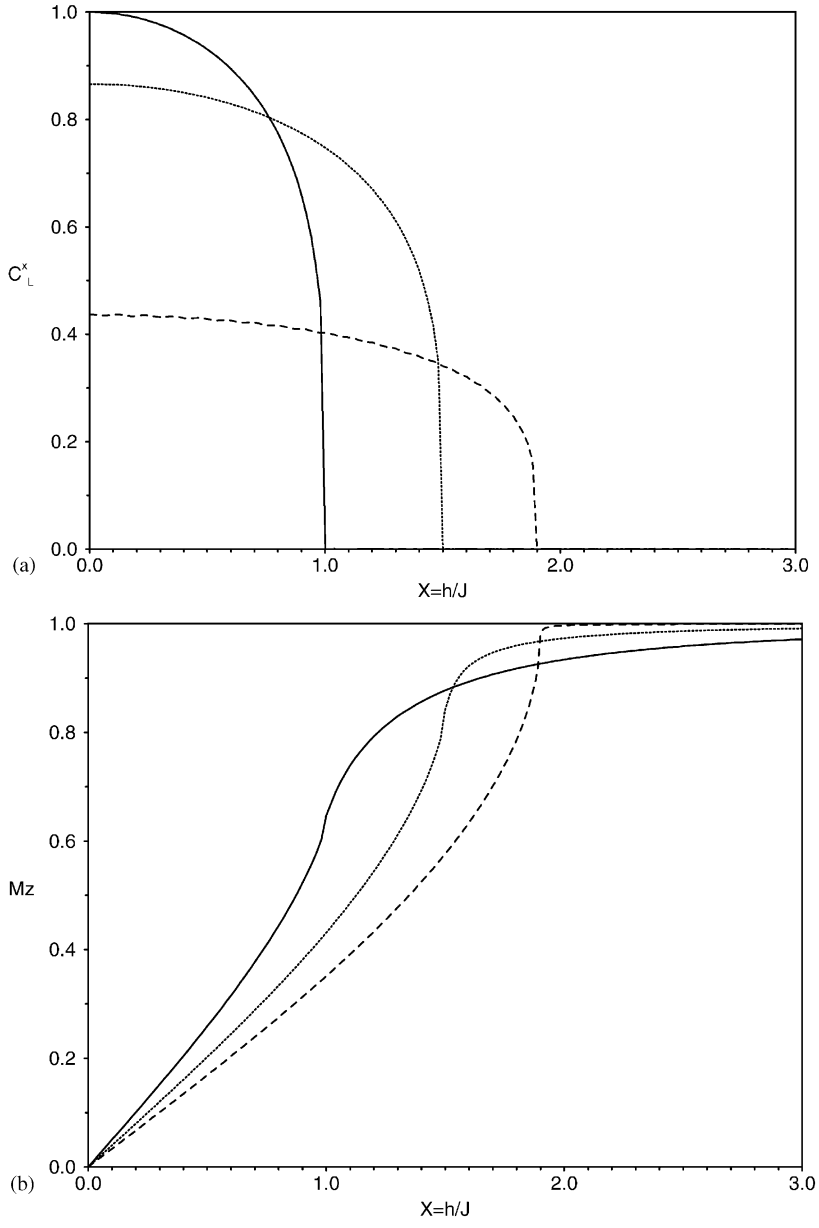

Fig. 1. The correlation function C_L^x (a) and order parameter M_z (b) of uniform chain as functions of $x = h/J$ for different α. The solid, dotted and dashed lines correspond to $\alpha = 0$, 0.5, and 0.9, respectively. The length of chain is 100.

In Fig. 3, we plot C_L^x and M_z of the period-three chain with 120 spins as functions of $x = h/J$ for different α, respectively. From Fig. 3, we can see that it undergoes a phase transition at the critical value for $0 < \alpha \leqslant \alpha_c(\gamma)$ and three phase transitions for $\alpha_c(\gamma) < \alpha < 1$. Also, the numerical results of the critical values are in good agreement with the analytical results.

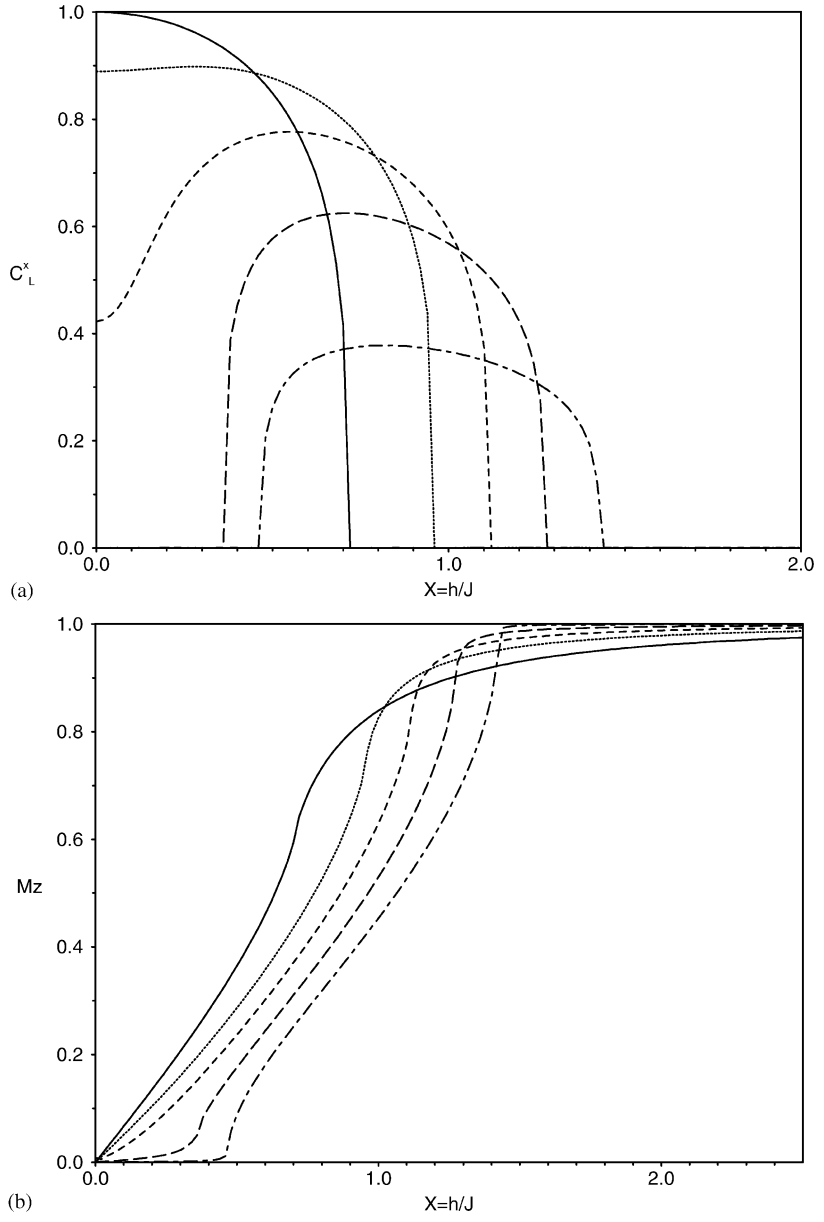

Fig. 2. The correlation function C_L^x (a) and order parameter M_z (b) of period-two chain as functions of $x = h/J$ for different α. The solid, dotted, short dashed, long dashed and dot-dashed lines correspond to $\alpha = 0$, 0.3, 0.5, 0.7 and 0.9, respectively. The length of chain is 128 and the $\gamma = 0.5$.

5. Conclusion and discussion

For the uniform chain, the quantum phase transition at $x_c = 1 + \alpha$ is similar as that of quantum Ising chain in a transverse field. That is, there are long range orders (LRO) between σ^x and σ^y when $h/J < x_c$ and the LRO of σ^x and σ^y disappear when $h/J > x_c$.

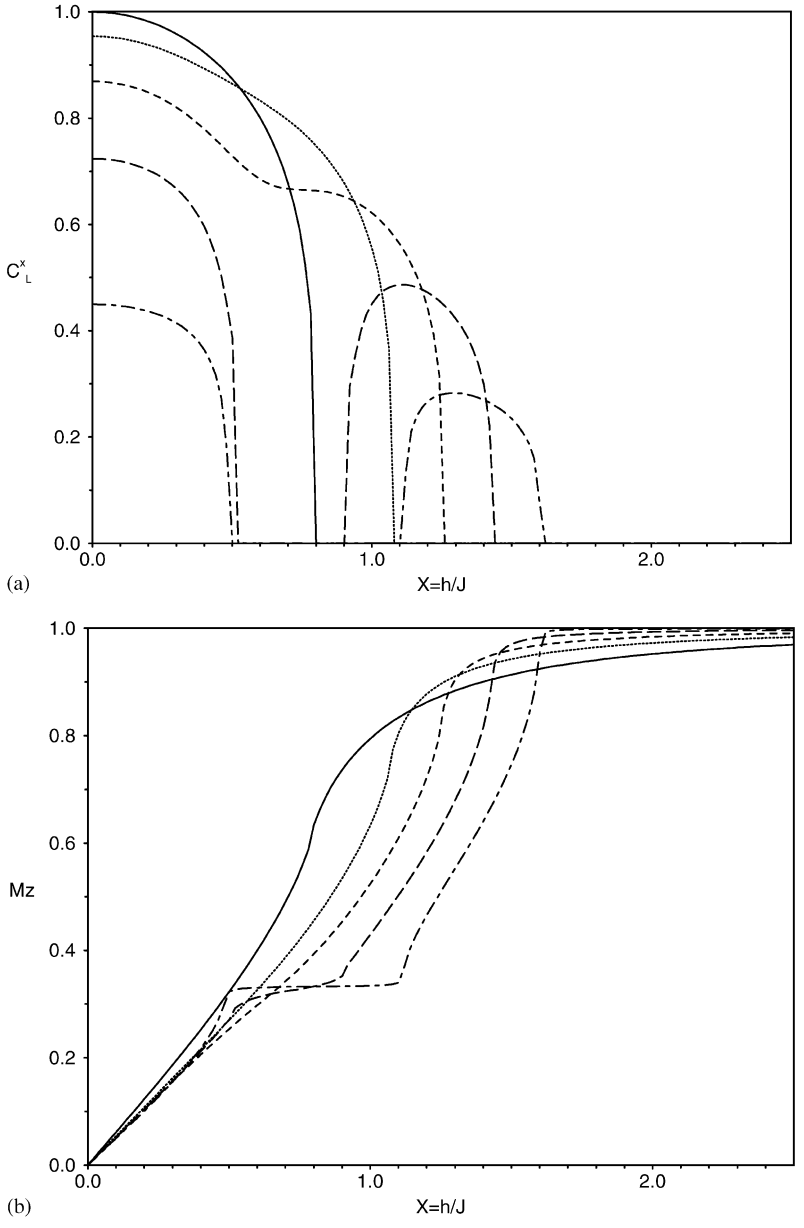

Fig. 3. The correlation function C_L^x (a) and order parameter M_z (b) of the period-three chain as functions of $x = h/J$ for different α. The solid, dotted, short dashed, long dashed and dot-dashed lines correspond to $\alpha = 0$, 0.3, 0.5, 0.7 and 0.9, respectively. The length of chain is 120 and the $\gamma = 0.5$.

For the period-two chain, there is phase transition at $h/J = x_{c_1}$ for any $0 < \alpha, \gamma < 1$. For $\gamma \to 1$, the periodic chain becomes a uniform chain and the $x_{c_1} = x_c$ and x_{c_2} become an imaginary number. Therefore, the quantum phase transition of the period-two chain at x_{c_1} is similar as that of the uniform chain and quantum Ising chain.

In order to understand the reason of quantum phase transition of the periodic chain at x_{c_2}, we consider the case of $\gamma \to 0$. When $\gamma = 0$, the chain breaks into groups of two-spin clusters. The Hamiltonian of two-spin system is

$$H = -\frac{J}{2}(\sigma_1^x \sigma_2^x + \alpha \sigma_1^y \sigma_2^y) - \frac{h}{2}(\sigma_1^z + \sigma_2^z). \tag{50}$$

In the space spanned by $\{|\uparrow\uparrow\rangle, |\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle, |\downarrow\downarrow\rangle\}$, the Hamiltonian is

$$H = \begin{pmatrix} -h & 0 & 0 & -\frac{J}{2}(1-\alpha) \\ 0 & 0 & -\frac{J}{2}(1+\alpha) & 0 \\ 0 & -\frac{J}{2}(1+\alpha) & 0 & 0 \\ -\frac{J}{2}(1-\alpha) & 0 & 0 & h \end{pmatrix}. \tag{51}$$

The eigenvalues of Hamiltonian (51) are

$$\lambda_{1,2} = \pm\frac{J}{2}(1+\alpha) \quad \text{and} \quad \lambda_{3,4} = \pm\sqrt{h^2 + \frac{J^2}{4}(1-\alpha)^2}. \tag{52}$$

The ground state of two-spin system is

$$\begin{aligned} &-\frac{J}{2}(1+\alpha) \quad \text{for } \frac{h}{J} < \sqrt{\alpha}, \\ &-\sqrt{h^2 + \frac{J^2}{4}(1-\alpha)^2} \quad \text{for } \frac{h}{J} > \sqrt{\alpha}. \end{aligned} \tag{53}$$

The wave function is

$$\left(0,\ \frac{1}{\sqrt{2}},\ \frac{1}{\sqrt{2}},\ 0\right) \tag{54}$$

for $h/J < \sqrt{\alpha}$ and

$$\left(\frac{J(1-\alpha)}{A},\ 0,\ 0,\ \frac{\sqrt{4h^2 + J^2(1-\alpha)^2} - 2h}{A}\right) \tag{55}$$

with $A = \sqrt{8h^2 + 2J^2(1-\alpha)^2 - 4h\sqrt{4h^2 + J^2(1-\alpha)^2}}$, for $h/J > \sqrt{\alpha}$, respectively.

Therefore, the ground state expected value of σ^z of two-spin cluster is

$$\bar{\sigma}_z = \left\langle \frac{1}{2}(\sigma_1^z + \sigma_2^z) \right\rangle = \begin{cases} 0 & \text{for } \frac{h}{J} < \sqrt{\alpha} \\ \frac{1}{A^2}[4h\sqrt{4h^2 + J^2(1-\alpha)^2} - 8h^2 0 & \text{for } \frac{h}{J} > \sqrt{\alpha} \end{cases} \tag{56}$$

From Eq. (56), we can find that the effective ground state spin of two-spin cluster consisted of two spins connected by interaction J that undergoes a transition at $h/J = \sqrt{\alpha}$ for $\gamma = 0$. In Fig. 4, we plot the effective ground state spin of two-spin cluster as functions of h/J for different α. For $\gamma > 0$, the critical value $(h/J)_c$ at which the effective ground state spin of two-spin cluster undergoes a sharp transition will change with γ. Therefore, the cluster effect is important for $\alpha > \gamma$ and the phase transition at $h/J = x_{c_2}$ is due to the change of effective spin of two-spin cluster. When $\alpha \leqslant \gamma$, the cluster effect is unimportant and there is only one transition point corresponding to $h/J = x_{c_1}$. These are confirmed by numerical results (see Fig. 2).

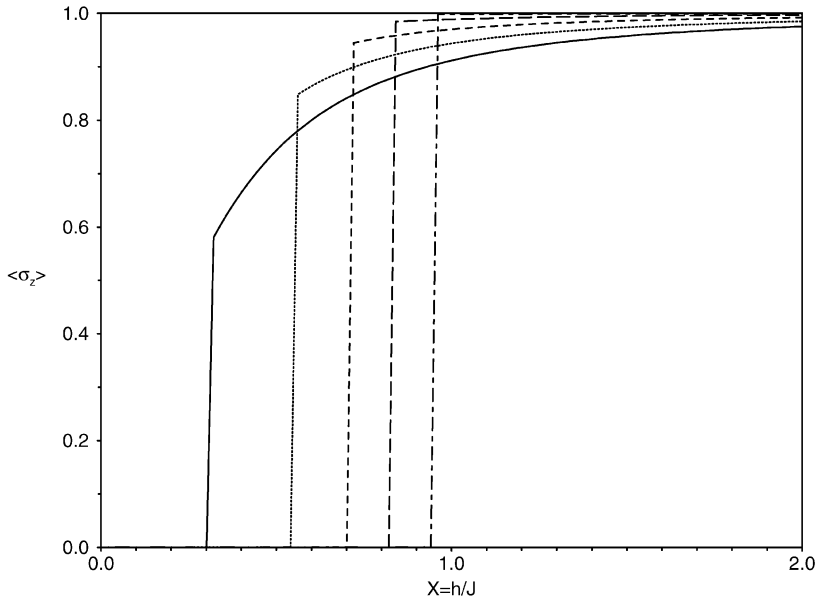

Fig. 4. The effective ground state spin of two-spin cluster as functions of h/J for different α. The solid, dotted, short dashed, long dashed and dot-dashed lines correspond to $\alpha = 0.1$, 0.3, 0.5, 0.7 and 0.9, respectively.

For the case of period-three chain, the chain breaks into group of three-spin clusters when $\gamma = 0$. The Hamiltonian of three-spin system is

$$H = -\frac{J}{2}[(\sigma_1^x\sigma_2^x + \sigma_2^x\sigma_3^x) + \alpha(\sigma_1^y\sigma_2^y + \sigma_2^y\sigma_3^y)] - \frac{h}{2}(\sigma_1^z + \sigma_2^z + \sigma_3^z). \tag{57}$$

In the space spanned by $\{|\uparrow\uparrow\uparrow\rangle, |\uparrow\downarrow\downarrow\rangle, |\downarrow\uparrow\downarrow\rangle, |\downarrow\downarrow\uparrow\rangle, |\downarrow\downarrow\downarrow\rangle, |\uparrow\uparrow\downarrow\rangle, |\uparrow\downarrow\uparrow\rangle, |\downarrow\uparrow\uparrow\rangle\}$

$$H = \frac{1}{2}\begin{pmatrix} -3h & -J\alpha_- & 0 & -J\alpha_- & 0 & 0 & 0 & 0 \\ -J\alpha_- & h & -J\alpha_+ & 0 & 0 & 0 & 0 & 0 \\ 0 & -J\alpha_+ & h & -J\alpha_+ & 0 & 0 & 0 & 0 \\ -J\alpha_- & 0 & -J\alpha_+ & h & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 3h & -J\alpha_- & 0 & -J\alpha_- \\ 0 & 0 & 0 & 0 & -J\alpha_- & -h & -J\alpha_+ & 0 \\ 0 & 0 & 0 & 0 & 0 & -J\alpha_+ & -h & -J\alpha_+ \\ 0 & 0 & 0 & 0 & -J\alpha_- & 0 & -J\alpha_+ & -h \end{pmatrix}. \tag{58}$$

with $\alpha_\pm = 1 \pm \alpha$. The lowest eigenvalue of Hamiltonian (58) is one of the roots of

$$E^3 - \frac{h}{2}E^2 - \left[\frac{5}{4}h^2 + (1+\alpha^2)J^2\right]E - \frac{3}{8}h^3 + \frac{3}{4}h(1+\alpha)^2J^2 - \frac{1}{4}(1-\alpha)^2hJ^2 = 0 \tag{59}$$

for small h/J and one of the roots of

$$E^3 + \frac{h}{2}E^2 - \left[\frac{5}{2}h^2 + (1+\alpha^2)J^2\right]E + \frac{3}{8}h^3 - \frac{3}{4}h(1+\alpha)^2J^2 + \frac{1}{4}(1-\alpha)^2hJ^2 = 0. \tag{60}$$

for large h/J and there is a transition at a critical x_0.

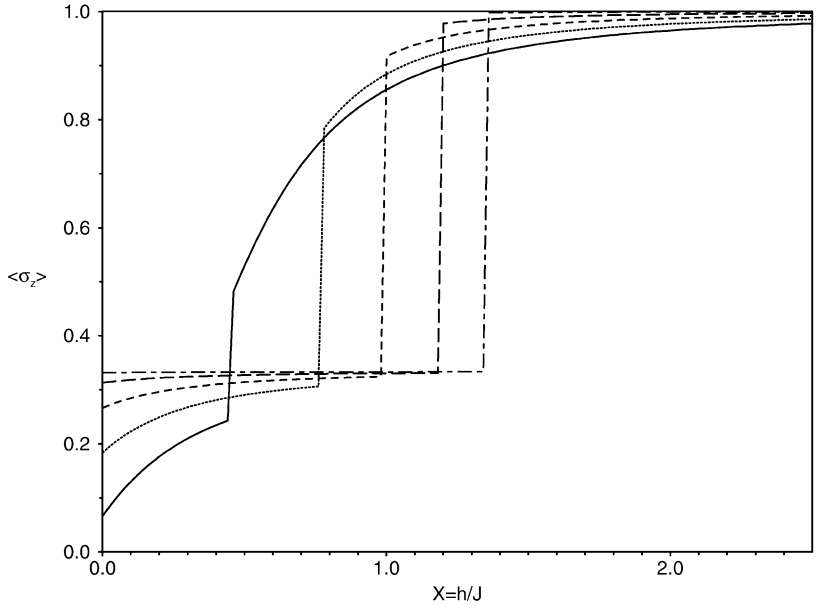

Fig. 5. The effective ground state spin of three-spin cluster as functions of h/J for different α. The solid, dotted, short dashed, long-dashed and dot-dashed lines correspond to $\alpha = 0.1$, 0.3, 0.5, 0.7 and 0.9, respectively.

Let E_+ and E_- denote the lowest roots of Eqs. (59) and (60), respectively. The eigenfunctions are

$$(0, 0, 0, 0, a_- b_-, b_-, c_- b_-, b_-) \tag{61}$$

for $x < x_0$ and

$$(a_+ b_+, b_+, c_+ b_+, b_+, 0, 0, 0, 0) \tag{62}$$

for $x > x_0$. Here $a_\pm = 2(1-\alpha)J/(\mp 3h - 2E_\pm)b_\pm$, $c_\pm = 2(1+\alpha)J/(\pm h - 2E_\pm)b_\pm$, and $b_\pm^2 = (a_\pm^2 + c_\pm^2 + 2)^{-1}$. Therefore, the effective ground state spin of three-spin cluster is

$$\bar{\sigma}_z = \begin{cases} \sigma_1 = \frac{1}{3}(1 - 4a_-^2 b_-^2) & \text{for } x < x_0, \\ \sigma_2 = \frac{1}{3}(4a_+^2 b_+^2 - 1) & \text{for } x > x_0. \end{cases} \tag{63}$$

Fig. 5 shows us the $\bar{\sigma}_z$ as functions of h/J. For $\gamma > 0$ and $\alpha > \alpha_c(\gamma)$, the effective ground state spin is σ_1 for small h/J and as h/J increases it undergoes a transition at $h/J = x_{c_1}$ which is similar to that in the uniform chain. For $x_{c_1} < h/J < x_{c_2}$, $M_z = \sigma_1$. At $h/J = x_{c_2}$, the effective ground state spin of three-spin cluster undergoes a transition. The transition at $h/J = x_{c_3}$ is similar to that at x_{c_1}. For $0 < \alpha < \alpha_c(\gamma)$, the situation is different. The critical value associated with the transition of the effective ground state spin of three-spin cluster is lower than the critical value corresponding to the transitions so that all effective spin σ_1 tends to be parallel to the external field. Therefore, the transitions at x_{c_1} and x_{c_2} disappear and there is only one transition at x_{c_3}. These are confirmed by numerical results (see Figs. 3a and b).

In conclusion, the transfer matrix method is used to study the quantum phase transitions of the uniform and periodic anisotropic XY quantum spin chain in a transverse field. It is found that there is only one quantum transition point for uniform chain at zero temperature. For periodic chain, there are more than one quantum phase transition point at some parameter region. The number of phase transition points depend on the parameters (α and γ) and structure of the systems. They are quite different from that of QI model, in which there is *only one* quantum phase transition point for all systems with periodic,

quasiperiodic and random structures. The critical values and the conditions of their existence are obtained analytically for period-two and three chains. The results are in good agreement with numerical results. These quantum phase transitions can be understood by considering the effects of clusters, resulting from competition between the property of period (γ) and anisotropy (α), and can be used to study the quantum transitions in random models. Also, we find that the transfer matrix method is very effective for the studies of these models and may be use to other more complex models.

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