Low Temperature Physics/Fizika Nizkikh Temperatur, 2021, vol. 47, No. 6, pp. 477–482

Quantum phase transitions in frustrated 1D Heisenberg spin systems

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Received February 8, 2021, published online April 26, 2021

A class of frustrated one-dimensional periodic Heisenberg spin systems formed either by triangular unit cells with spin 1/2 or by composite unit cells formed by two different structural units, triangles and small linear segments formed by an odd number of spin-1/2 is investigated. Based on perturbative processing and numerical calculations of the density matrix renormalization group method, the gapless character of the exact energy spectrum of excitation for these systems was found. Their instability with respect to regular (Peierls) oscillations of interactions between structural units is demonstrated. The corresponding critical exponents for the energies of the ground state are estimated numerically. For some frustrated systems, a quantum phase transition associated with the spin symmetry of the ground state, caused by frustration, has been discovered.

Keywords: Heisenberg spin Hamiltonian, frustrated one-dimensional spin systems, quantum phase transitions.

1. Introduction

The theoretical study of the peculiarities of the energy spectrum and magnetic properties of one-dimensional (1D) Heisenberg spin systems with antiferromagnetic coupling between neighboring spins is motivated by a large number of successful applications of Heisenberg spin Hamiltonian to the simulation of the magnetic properties of polymeric transition-metal complexes [1–3], organic polymers with conjugated bonds [4–6], stackings of radicals [7]; crystals of ion-radical salts [8, 9]; and so on.

The lowest excitations of the 1D periodic bipartite Heisenberg spin-1/2 systems having the odd number of spins n per unit cells obey the extended Lieb–Schultz–Mattis (LSM) theorem [10–12] according to which, these excitations are gapless, in the limit of long chains. In contrast, the systems with even n like a two-leg spin ladder usually have gapped excitation energy spectra. Therefore, the study of periodic spin systems which have gapless excitation spectrum and even numbers of spins per unit cell is of interest.

In our previous paper [13], we studied several 1D bipartite periodic spin systems with composite unit cells with even n. As expected, these showed no gap in the exact energy spectrum, for the long-chain limit.

Here we continue such a study to extend our consideration to the case of 1D periodic spin systems with *geometrical frustrations*. In particular, in Sec. 2 we study the case of weak interaction between triangular unit cells or between structural units of the corresponding composite unit cells of our systems. The (nonequilateral) isosceles triangles of spin-1/2 have the nondegenerate ground state. This permits us to apply simple perturbative analysis of the lowest energy states of the corresponding frustrated systems similar to bipartite 1D systems from [13]. We demonstrate here the gapless character of the lowest part of the exact energy spectrum, which results in instability of the corresponding magnets against the periodic lattice distortions such as spin-Peierls transition (known for the simple strictly 1D chain, with $n = 1$). The case of equilateral triangles is more complicated due to the double degeneracy of the corresponding ground state of this triangle. Hence, we may expect, that the transition from isosceles triangles to equilateral ones due to the variation of the corresponding coupling parameters may result in significant changes in the lowest part of the energy spectrum and the magnetic properties of the frustrated systems. The perturbative analysis of the energy spectra of such spin systems also demonstrate the existence of gapped excitations which result in an intermediate plateau in field dependence of the

magnetization at low temperatures. In Section 3 we extended the above consideration to the case of intermediate values of coupling between the unit cell and structural units by means of the numerical density matrix renormalization group method (DMRG) [14].

2. Perturbation theory

One of the simplest representatives of 1D frustrated spin-1/2 systems is the chain of interacting isosceles triangles. There are also a bit more complicated chain systems with composite unit cells formed by two structural units: isosceles triangle and the finite fragment of a linear spin-1/2 chain, as shown below in Fig. 1.

The corresponding spin Hamiltonians can be written in the form

$$\mathcal{H} = \sum_{i=1}^{N} H_n(i) + J \sum_{i=1}^{N-1} S_{i,n} S_{i+1,1}, \qquad (1)$$

where N is the total number of unit cells of the corresponding spin chain system, n is the total number of spin-1/2 sites of the unit cell ($n = 3$, 4, 6 for the systems 1(a), 1(b), and 1(c), respectively), $S_{i,j}$ is the spin-1/2 operator located on the jth site of the ith unit cell.

$$H_3(i) = J_0 S_{i,2}(S_{i,1} + S_{i,3}) + J_1 S_{i,1} S_{i,3},$$

$$H_4(i) = H_3(i) + J S_{i,3} S_{i,4},$$

$$H_6(i) = H_4(i) + J_0 S_{i,5}(S_{i,4} + S_{i,6}).$$

In our study the coupling constants J, J_0, and J_1 take the non-negative values only.

We view each unit cells in Figs. 1(b) and 1(c) to be composed of two primitive cells: a triangular one and a second either of 1 or 3 vertices. At $J_0 \neq J_1$ the ground state of triangular primitive unit cell is double degenerate with respect to z projection of total spin m and the corresponding wave functions have the form:

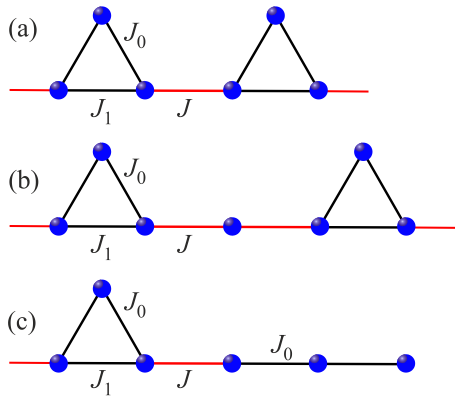

Fig. 1. (Color online) The fragments of the chain of interacting spin-1/2 triangles and two 1D spin systems with composite unit cells.

$$\varphi_0(m) = \begin{cases} (2\alpha\beta\alpha - \alpha\alpha\beta - \beta\alpha\alpha)/\sqrt{6}, & m = 1/2 \\ (2\beta\alpha\beta - \beta\beta\alpha - \alpha\beta\beta)/\sqrt{6}, & m = -1/2 \end{cases}, \quad \text{at } J_0 > J_1$$

and

$$\phi_0(m) = \begin{cases} (\alpha\alpha\beta - \beta\alpha\alpha)/\sqrt{2}, & m = 1/2 \\ (\beta\beta\alpha - \alpha\beta\beta)/\sqrt{2}, & m = -1/2 \end{cases}, \quad \text{at } J_0 < J_1.$$

Here α and β are the eigenvectors of spin-1/2 operator S_i^z.

As a result, the set of N noninteracting isosceles triangles has 2^N degenerate ground state. In particular, for the case $J_0 > J_1$ the corresponding wave functions have the form

$$\Psi\{M\} = \prod_{i=1}^{N} \varphi_{0,i}(m_i), \quad m = \pm 1/2, \quad M = \sum_{i=1}^{N} m_i.$$

For equilateral spin triangle ($J_0 = J_1$) we have additional degeneracy of the unit cell ground state with respect of C_{3v} space symmetry of the triangle

$$\begin{cases} \theta^+(m) = [\varphi_0(m) + i\phi_0(m)]/\sqrt{2} \\ \theta^-(m) = [\varphi_0(m) - i\phi_0(m)]/\sqrt{2} \end{cases}$$

and the corresponding system of non-interacting triangles has 4^N degenerate ground state.

The interaction between neighbor unit cells in the chain systems, shown on Fig. 1, resolves the above degeneracy. For the case $J_0 - J_1 \gg J$ it can be shown similar to [13] that the lowest part of the energy spectrum of above spin chain models can be described by means of the first order of the perturbation theory (PT) in the coupling J. The corresponding low-energy Hamiltonians may we have written in a general form as the Hamiltonian of antiferromagnetic uniform spin-1/2 chain:

$$\mathcal{H} = N\varepsilon_0 + J_{\text{eff}} \sum_{i=1}^{N-1} S_i S_{i+1}. \qquad (2)$$

Here for the Fig. 1(a) N is the total number of triangular unit cells, ε_0 is the ground state energy of isolated unit cell $\left(\varepsilon_0 = -J_0 + \frac{1}{4} J_{\text{eff}}\right)$ and $J_{\text{eff}} = 4J/9$. For the Figs. 1(b) and 1(c) N is the total number of structural units, ε_0 is the mean ground state energy of isolated structural unit and J_{eff} equals to $2J/3$ and $4J/9$ for the systems 1(b) and 1(c), respectively.

According to above PT consideration, for $J_0 - J_1 \gg J$ the systems 1(a)–1(c) have non-degenerate singlet ground state. In addition, in the limit $N \to \infty$ they have the gapless excitation energy spectrum. Similar to the chain systems considered in [13], the gapless energy spectrum of (2) leads to the spin-Peierls instability of the above 1D spin systems with the critical exponent for the ground state energy $\alpha \approx 1.45$ [9]. In other words we universal critical behavior of our spin systems at $J_0 - J_1 \gg J$ despite the even number of spin-1/2 per unit cells for systems 1(b) and 1(c).

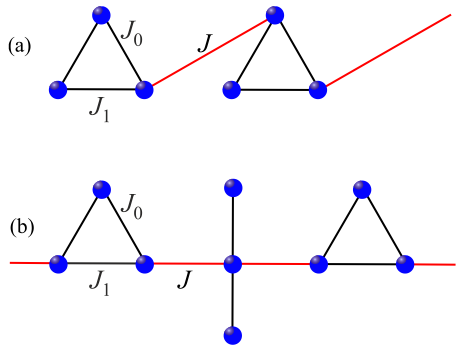

Fig. 2. (Color online) The fragments of two 1D frustrated spin systems of "branched" geometry.

At $J_0 = J_1$, the case of weakly interacting unit cells can be also studied by the first order of PT in coupling J similar to [15], but the corresponding low-energy Hamiltonians have more complicated structure and require additional numerical treatment. Therefore we skip here the corresponding PT analysis and consider the case of weakly interacting equilateral triangles by the direct DMRG calculations in the next section. For $J_1 - J_0 \gg J$ the degeneracy of the energy spectra of our systems is lifted only in the second PT order in J. In other words, we may expect a significant change of the exact energy spectrum of the systems 1(a)–1(c) at the transition from isosceles triangles to equilateral one.

Now, let us consider the following 1D frustrated spin systems presented in Fig. 2.

For the case of $J_0 - J_1 \gg J$ the first PT order in J give the following low-energy effective spin-1/2 Hamiltonians:

System 2(a)

$$\mathcal{H} = -N\left(J_0 - \frac{1}{4}J_1\right) - \frac{2}{3}J\sum_{i=1}^{N-1} S_i S_{i+1}. \qquad (3)$$

System 2(b)

$$\mathcal{H} = -N\left(2J_0 - \frac{1}{4}J_1\right) - \frac{2}{3}J\sum_{i=1}^{2N-1} S_i S_{i+1}. \qquad (4)$$

Here N is the total number of unit cells.

Both the Hamiltonians (3) and (4) have macroscopic ground state spin $S = N/2$ and $S = N$, respectively. In case of $J_1 = 0$, this result is in agreement with the extended LSM theorem due to bipartite character of the corresponding spin lattices. We also have gapless energy spectrum for both systems. Nevertheless, for $J_0 - J_1 \gg J$, in contrast to the systems shown on Fig. 1, the systems 2(a) and 2(b) should be stable against spin-Peierls transition because of the absence of the excitations with the spin $S = S_0$.

Note also, that similar to the bipartite spin systems considered in [13], our frustrated system at $J_0 - J_1 \gg J$ have two types of the excitations. First one is described by the effective Hamiltonians (2)–(4) and has gapless character. It corresponds the excitations with the total spin $0 \le S < N/2$. The second type corresponds to the gapped excitations with $S > N/2$. In the result, our spin systems should have at least one intermediate plateau in the field dependence of its magnetization at low temperatures.

3. Numerical simulation

In order to extend our analysis on the case of arbitrary positive values of coupling parameters, we used two versions of the DMRG method, so-called finite and infinite algorithms. In addition, for the infinite algorithm, we used structural units of the corresponding spin chain systems as the active blocks similar to [16]. For simplicity, we put $J_0 = 1$ in all numerical calculations.

Let us start the consideration of the results of our numerical study from the system 1(a). According to our DMRG study, this spin system has the nondegenerate singlet ground state and the gapless lowest excitations at arbitrary positive value of coupling constants J_1 and J. Hence, the infinite system 1(a) may be unstable against periodic lattice distortions of the distances between neighbor triangles (spin-Peierls instability). To study this instability, we used a modified Hamiltonian (2) with oscillating values of coupling between unit cells with the numbers i and $i+1$

$$J(i) = J\left(1 + (-1)^i \delta\right), \quad \delta \ll 1. \qquad (5)$$

In case of spin-Peierls instability, the ground state energy $E_0(\delta)$ of modified Hamiltonian (2) should be non-analytical function of the distortion parameter δ. For the systems with the open ends the quantity $\Delta E = E_0(\delta) + E_0(-\delta) - 2E_0(0)$ does not depend on the sign of δ. Similar to [13] non-analytical behavior of the ground state energy in thermodynamic limit is associated with the dependence $\Delta E \sim |\delta|^{\alpha}$, $1 \le \alpha < 2$. We used the DMRG

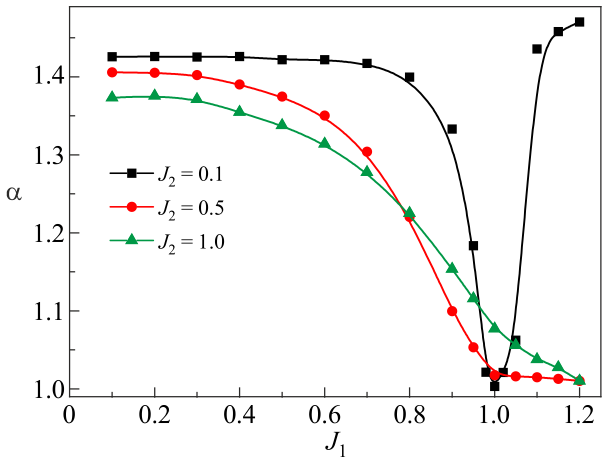

Fig. 3. The dependence $\alpha(J_1)$ for the spin system 1(a) at three different values of the interaction between neighbor unit cells.

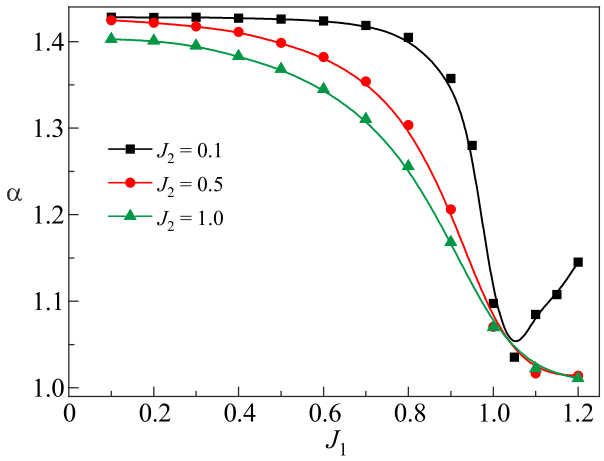

Fig. 4. The dependence $\alpha(J_1)$ for the spin system 1(b) at three different values of the interaction between neighbor unit cells.

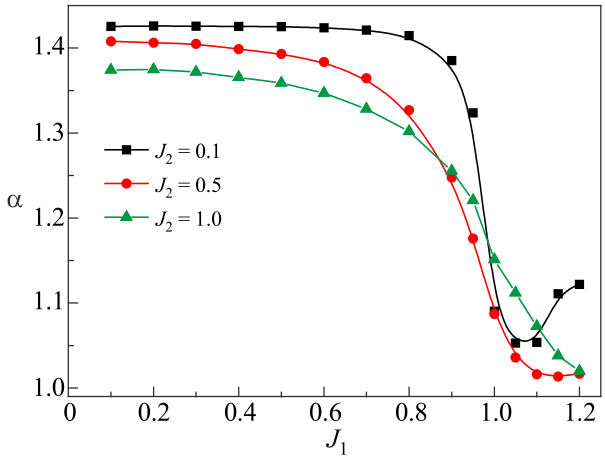

Fig. 5. The dependence $\alpha(J_1)$ for the spin system 1(c) at three different values of the interaction between neighbor unit cells.

method to calculate the value $E_0(\delta)$ for five different values of the small parameter δ. To reach proper accuracy, we used 50 optimized states and extrapolated our numerical results to the infinite spin system.

As for exact energy spectra and critical behavior of the frustrated spin systems with composite unit cells 1(b) and 1(c), our DMRG study gave the results, which are very similar to the case of the system 1(a). Both systems have the gapless energy spectra despite the even number of spin-1/2 per unit cell. In both cases, the critical exponents for the ground state energy take the values less than 2, which mean the instability of the systems against to the transition into the state with periodic oscillations of the coupling between structural units. It should be noted, that in contrast to the system 1(a) the above transition does not change the space symmetry of the systems 1(b) and 1(c).

The results of our numerical estimations of the values of critical exponents for the above spin systems are presented of Figs. 3–5. It is of interest significant decrease of the value of critical exponents in the vicinity of the point of strong frustration $J_1 = 1$ for all the systems studied.

According to our preliminary PT study of the chain systems 2(a) and 2(b) it has macroscopic ground state spin at $J_0 - J_1 \gg J$. For intermediate values of coupling J the ground state spin S_0 may change its value. We performed the exact diagonalization study of the lowest energy states of finite lattice clusters containing up to 18 spins in subspaces with specified values of total spin (see Fig. 6).

This study demonstrated for both clusters the quick decrease of the ground state spin from the value S_0 to zero one in the vicinity of some critical value of coupling J_1^*.

We also performed the corresponding DMRG calculations in subspaces with specified values of z-projection of total spin, which are support the above conclusion. Moreover, for system 2(a) of a big size we may suppose the presence of jumpwise transition from the state with $S_0 = N/2$ at $J_1 < J_1^*$ to the state with $S_0 = 0$ at $J_1 > J_1^*$ for given value of coupling J between triangular unit cells (see Fig. 7).

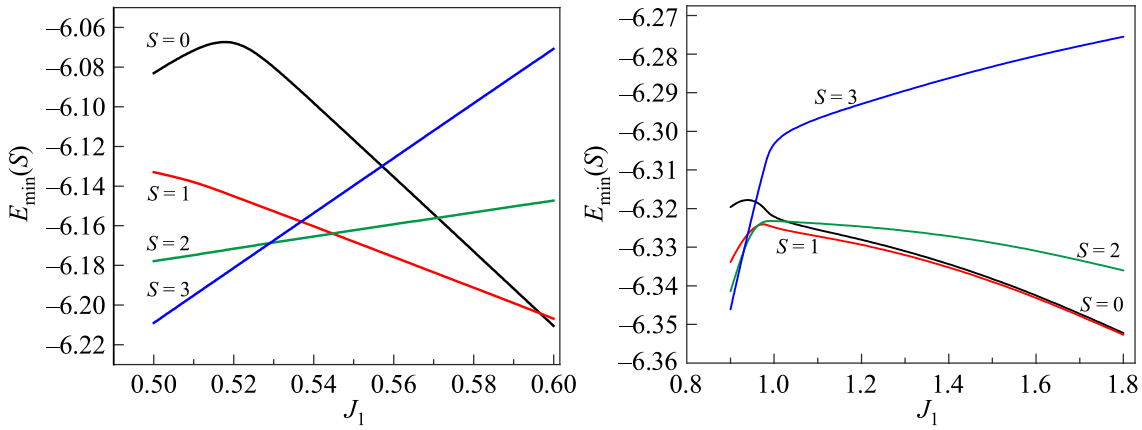

Fig. 6. The lowest energy states of finite lattice clusters of the systems 2(a) and 2(b) (left and right figures, correspondingly) containing 18 spins.

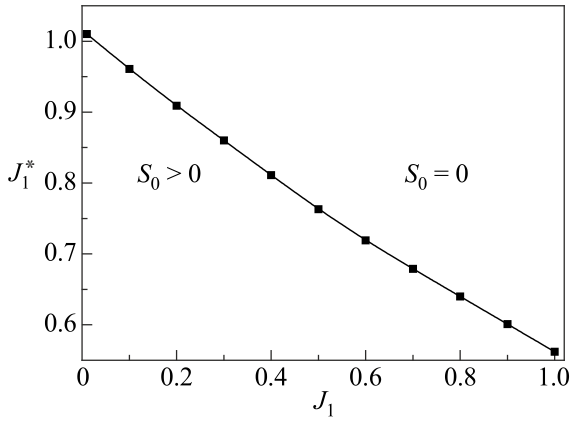

Fig. 7. Critical value of frustration parameter J_1^* vs interaction between neighbor unit cells J of the system 2(a).

Note also that at $J_1 = 1$ the systems 1(a) and 2(a) have coincident energy spectrum at any values of J, which corresponds to the absence of the transition with the change of the ground state spin.

According to our DMRG study at $J_1 < J_1^*$ we have quadratic dependence of the ground state energy on the value of distortion parameter δ (critical exponent $\alpha \sim 2$), which corresponds to the absence of spin Peierls instability. At $J_1 > J_1^*$ we found rapid decrease of the value of critical exponent up to the value $\alpha \sim 1$ at $J_1 = 1$ similar to the case of the systems 1(a)–1(c).

The presence of the transition with the quick change in the ground state spin for the systems 2(a) and 2(b) gives the peculiarity in its magnetization profile at low temperatures. Unfortunately, quantum Monte-Carlo method is not applicable to study the low-temperature thermodynamics of these frustrated spin systems. That is why we used DMRG numerical simulation to obtain zero-temperature magnetization profile for the systems 2(a)–2(b). The results are presented in Fig. 8. The dependencies $m(h)$ clearly demonstrate the presence of intermediate magnetization plateau, which is in agreement with our preliminary perturbative treatment and known results for 1D for bipartite spin systems with the macroscopic ground state spin [16, 17]. It is of interest that for model 2(a) the size of this plateau decreased with the increase of the coupling constant J_1.

4. Conclusions

Several one-dimensional models of frustrated spin with unit cells formed by odd and even spin-1/2 have been proposed. These spin models are characterized by the gapless character of the exact energy spectrum of the corresponding Heisenberg spin Hamiltonians. It should be noted that the gapless structure of energy spectrum of similar frustrated systems was discovered earlier [18–21], but in these papers the case equilateral triangles (i.e., $J_0 = J_1$) was not considered. Using perturbation theory and numerical simulation by means of DMRG method we studied the possible instability of the corresponding magnets against the periodic lattice distortions like spin-Peierls transition. It was found that for our two models with a “branched” geometry, there is a transition from a stable spin system to an unstable one, mediated by the magnitude of the spin coupling, which is responsible for their frustrated nature. For unstable one-dimensional spin systems, a numerically significant decrease in the value of the critical exponent for the ground-state energy in the vicinity of the point of strong frustration was found in comparison with similar two-part one-dimensional spin models. For our “branched” spin models, the existence of quantum phase transitions associated with a change in the spin symmetry of the ground state was also numerically discovered, and the corresponding set of critical values of the coupling parameter responsible for the effects of frustration was estimated.

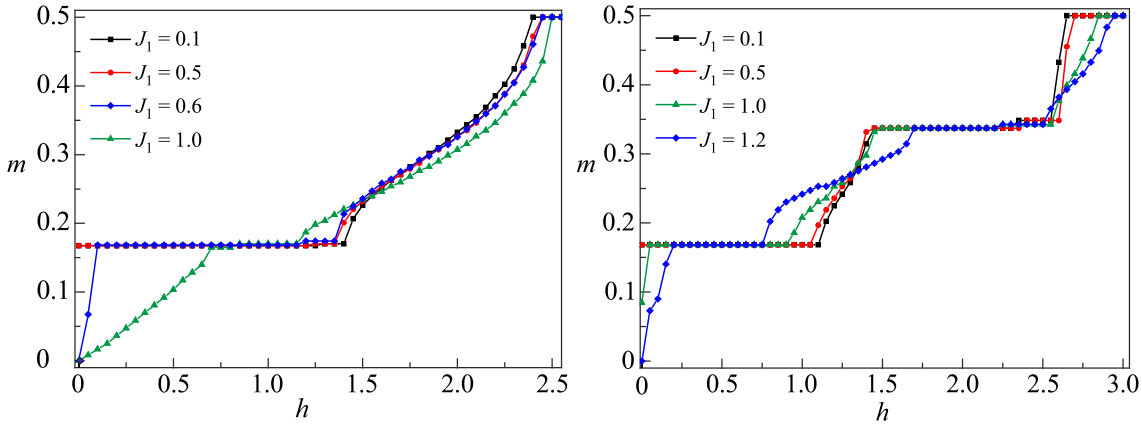

Fig. 8. (Color online) The field dependence of zero-temperature specific magnetization of the systems 2(a) and 2(b) (left and right figures, correspondingly) at four different values of J_1. Exchange constant $J = 1$ for all these curves.

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Квантові фазові переходи у фрустрованих одновимірних спінових системах Гейзенберга

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Досліджено клас фрустрованих одновимірних періодичних спінових систем Гейзенберга, які утворені або трикутними елементарними комірками зі спіном 1/2, або складовими елементарними комірками з двох різних структурних одиниць: трикутників та невеликих лінійних сегментів, які сформовані непарним числом спінів 1/2. За допомогою теорії збурень та чисельних розрахунків, а також методу ренормалізаційної групи матриці густини, знайдено безщілинний характер точного енергетичного спектра збудження для цих систем. Продемонстровано їх нестійкість відносно до регулярних (пайєрлсовських) коливань взаємодій між структурними одиницями. Чисельно оцінено відповідні критичні показники щодо енергій основного стану. Для деяких фрустрованих систем виявлено квантовий фазовий перехід, який пов’язаний зі спіновою симетрією основного стану, обумовленого фрустрацією.

Ключові слова: спіновий гамільтоніан Гейзенберга, фрустровані одновимірні спінові системи, квантові фазові переходи.