MULTICRITICAL POINT IN THE ONE-DIMENSIONAL QUANTUM COMPASS MODEL

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The one-dimensional spin-1/2 quantum compass model is considered. There is a multicritical point in the ground state magnetic phase diagram of the model. By using the Jordan–Wigner transformation the diagonalized Hamiltonian is obtained and analytic expressions for the spin–spin correlation functions are determined at the multicritical point. On the other hand, the critical exponent of the energy gap in the vicinity of the multicritical point is calculated by a practical finite size scaling approach.

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1. Introduction

Commensurate–incommensurate (C-IC) phase transitions have been discovered to have many interesting properties and can be characterized by parameters known as critical exponents. In the ground state phase diagram of any system containing different phases, there exists a special combination of parameters, known as the critical point, at which the transition between two phases becomes a C-IC phase transition. The C-IC phase transitions arising in different systems often possess the same set of critical exponents which is called the universality.

Multicritical points are special points in the ground state phase diagram of some systems with a C-IC phase transition. At least two parameters must be adjusted to reach a multicritical point. It is expected that, at a multicritical point, the system belongs to a universality class different from the normal universality class.

Low-dimensional spin systems are good candidate for studying the C-IC phase transitions. In particular, we consider the 1D spin-1/2 quantum compass model [1–7]. In fact, the quantum compass model is defined for explaining the low-temperature behavior of some Mott insulators. In this

model, the orbital degrees of freedom are represented by (pseudo)spin-1/2 operators and coupled anisotropically in such a way that they mimic the competition between orbital ordering in different directions. By mapping the model to a quantum Ising chain, an exact solution for the ground state energy and the complete excitation spectrum are obtained [1]. It is shown that the 1D quantum compass model exhibits a first-order phase transition between two disordered phases with opposite signs of certain local spin correlations. The model is also diagonalized exactly by a direct Jordan–Wigner transformation [3]. The obtained by latter approach results, confirm the existence of the first-order phase transition in the ground state phase diagram. In a very interesting work [5], it is found that the reported first-order phase transition, in fact, occurs at a multicritical point, where a line of the first-order transition meets with a line of the second-order transition. Based on a numerical analysis [6], the first and second order quantum phase transitions in the ground state phase diagram have been identified. The effect of a transverse magnetic field on the 1D quantum compass model is also well studied recently [8–13].

In the present work, we consider the 1D quantum compass model and study the system at the multicritical point. First, by mapping the model to the spin-1/2 XY chain [14, 15], we calculate the spin–spin correlation functions at the multicritical point. Then, applying a practical finite size scaling approach, we investigate the critical exponents of the energy gap, the ground and first excited state energies in vicinity of the multicritical point.

The paper is organized as follows. In the forthcoming section, we present our analytical results on the spin–spin correlation functions at the multicritical points. In Section 3, the numerical part of the work on deriving the critical exponents is explained. Finally, in Section 4, we conclude and summarize our results.

2. Correlation functions at the multicritical point

The Hamiltonian of the 1D quantum compass model with periodic boundary conditions is defined as [5]

$$\mathcal{H} = \sum_{j=1}^{N'} \left(J_1 \sigma_{2j-1}^x \sigma_{2j}^x + J_2 \sigma_{2j-1}^y \sigma_{2j}^y + L \sigma_{2j}^x \sigma_{2j+1}^x \right) , \tag{1}$$

where $\sigma_j^{x,y}$ are the Pauli operators on the jth site and J_1, J_2, L are the exchange couplings $N = 2N'$ is the number of spins. The ground state phase diagram of the model is very rich including four different gapped phases which are separated with the first-order ($J_1/L = 0$) and the second-order

($J_2/L = 1$) critical lines [5, 6]. The point where the line of the first-order transition ($J_1/L = 0$) meets with a line of the second-order ($J_2/L = 1$) transition is called the multicritical point. This Hamiltonian at the multicritical point can be rewritten as

$$\mathcal{H} = J \sum_{j=1}^{N'} \left(\sigma_{2j-1}^{y} \sigma_{2j}^{y} + \sigma_{2j}^{x} \sigma_{2j+1}^{x} \right) , \tag{2}$$

where $J = J_2 = L$. Mapping the spin-$\frac{1}{2}$ operators onto Fermi operators by means of the Jordan–Wigner transformation

$$\begin{aligned} S_{2j-1}^{+} &= a_j^{\dagger} \, e^{i\pi \left(\Sigma_{m=1}^{j-1} a_m^{\dagger} a_m + \Sigma_{m=1}^{j-1} b_m^{\dagger} b_m \right)} , \\ S_{2j}^{+} &= b_j^{\dagger} \, e^{i\pi \left(\Sigma_{m=1}^{j} a_m^{\dagger} a_m + \Sigma_{m=1}^{j-1} b_m^{\dagger} b_m \right)} , \end{aligned} \tag{3}$$

the quantum compass model at the multicritical point is transformed to a 1D noninteracting spinless fermion system as

$$\mathcal{H} = J \sum_{j=1} \left(a_j^{\dagger} b_j + b_j^{\dagger} a_j - a_j^{\dagger} b_j^{\dagger} - b_j a_j + b_j^{\dagger} a_{j+1}^{\dagger} + b_j^{\dagger} a_{j+1} + a_{j+1}^{\dagger} b_j + a_{j+1} b_j \right) . \tag{4}$$

By a Fourier transformation, $a_j^{\dagger} = \frac{1}{\sqrt{N'}} \Sigma_k a_k^{\dagger} e^{ikj}$, the Hamiltonian Eq. (4) is simplified as

$$\begin{aligned} \mathcal{H} &= \sum_{k>0} A \left(a_k^{\dagger} b_k + b_{-k}^{\dagger} a_{-k} - a_k^{\dagger} b_{-k}^{\dagger} - b_k a_{-k} \right) \\ &\quad + \sum_{k>0} A^{*} \left(b_k^{\dagger} a_k + a_{-k}^{\dagger} b_{-k} - a_{-k}^{\dagger} b_{-k}^{\dagger} - b_{-k} a_k \right) , \end{aligned} \tag{5}$$

where $A = J(1 + e^{ik})$. Using the following unitary (or Bogoliubov) transformations

$$\begin{aligned} a_k &= \sqrt{\frac{A}{\varepsilon_k}} \left(\alpha_k + \beta_{-k}^{\dagger} \right) , \\ b_k &= \sqrt{\frac{A^{*}}{\varepsilon_k}} \left(\alpha_k - \beta_{-k}^{\dagger} \right) , \end{aligned} \tag{6}$$

the diagonalized Hamiltonian is given by

$$\mathcal{H} = \sum_{k} \left(\alpha_k^{\dagger} \alpha_k - 1/2 \right) \varepsilon_k , \tag{7}$$

where $\varepsilon_k = 2\sqrt{AA^*}$ is the energy spectrum. However, as is seen, only states with even or odd numbers of Bogoliubov quasiparticles belong to the physical spectrum of the Hamiltonian in the multicritical point [1].

Using the diagonalized form, one can find a general form for the spin–spin correlation functions at the multicritical point as

$$\begin{aligned} \left\langle \sigma^x_{2j-1}\sigma^x_{2j-1+2n}\right\rangle &= \left\langle \sigma^y_{2j-1}\sigma^y_{2j-1+2n}\right\rangle = 0\,, \\ \left\langle \sigma^x_{2j}\sigma^x_{2j+2n}\right\rangle &= \left\langle \sigma^y_{2j}\sigma^y_{2j+2n}\right\rangle = 0\,, \\ \left\langle \sigma^x_{2j-1}\sigma^x_{2j+2n}\right\rangle &= \left\langle \sigma^y_{2j-1}\sigma^y_{2j+2n}\right\rangle = -\frac{2}{\pi}\left[\frac{(-1)^n}{1+2n}\right]. \end{aligned} \tag{8}$$

We emphasize that the spins in the quantum compass model are not correlated along the z direction. We have to mentioned that the spin–spin correlation functions only for the nearest neighbor spins have been calculated [1] as $\langle \sigma^y_{2j-1}\sigma^y_{2j}\rangle = \langle \sigma^x_{2j}\sigma^x_{2j+1}\rangle = -\frac{2}{\Pi}$, which confirms our results (Eq. (8)).

3. Gap exponent in the vicinity of the multicritical point

The finite size scaling method is an efficient way for extracting critical exponents from finite-size systems results [16, 17]. In this method, one should compare a sequence of finite lattices. The finite lattice systems are solved exactly, and various quantities can be calculated as a function of the lattice size N, for small values of N. Finally, these functions are scaled up to $N \longrightarrow \infty$. Two steps are needed before these ideas can be realized. First, one needs a procedure for solving the finite lattice systems exactly. Second, one needs a procedure for extrapolating from finite to infinite N. In the step one, we have used the numerical Lanczos method to obtain the energy gap. We recognized the energy gap as the difference between the first and the ground state energies in finite chains and also did not find any irregular size dependence in our numerical results.

Using the Lanczos method, we have computed the energy gap as a function of the chain length N and the different values of the exchange parameter J_1 very close to the multicritical point (please note that we have considered $\frac{J_2}{L} = 1 - \frac{J_1}{L}$). We have implemented the Lanczos algorithm on finite size chains $N = 8, 12, 16, 20, 24$ by using periodic boundary conditions. The energy gap as a function of the chain length N and exchange J_1 is defined as

$$G(N, J_1) = E_1(N, J_1) - E_0(N, J_1)\,, \tag{9}$$

where $E_0(N, J_1)$ and $E_1(N, J_1)$ are the ground and first excited energies. At the multicritical point ($J_1 = 0$), the spectrum is gapless. When the

exchange J_1 is added, a non zero gap develops and in the thermodynamic limit behaves as

$$G(J_1) \propto J_1^{\nu}\,, \qquad J_1 \longrightarrow 0\,, \tag{10}$$

where ν is the critical exponent of the energy gap. With our Lanczos scheme we can compute $G(N, J_1)$, which approaches $G(J_1)$ when N is large. We write the scaling function $f(x)$ as the following expression

$$N\,G(N, J_1) = N\,\left(E_1(N, J_1) - E_0(N, J_1)\right) = f(x)\,, \tag{11}$$

where $x = NJ_1^{\nu}$ is a scaling parameter. As expected, the behavior of this equation in the combined limit

$$N \longrightarrow \infty\,, \qquad J_1 \longrightarrow 0 \quad (x \gg 1) \tag{12}$$

is consistent with Eq. (10). Thus, it can be assumed that the asymptotic form of the scaling function is

$$f(x) \sim x^{\phi} \tag{13}$$

and the ϕ-exponent in the large-x regime, $x \gg 1$, must be equal to one ($\phi = 1$). Then we get in the large-x regime

$$\lim_{N \longrightarrow \infty (x \gg 1)} f(x) = N\,(E_1(N, J_1) - E_0(N, J_1)) \sim x\,. \tag{14}$$

This equation shows that the large-x behavior of the scaling function $f(x)$ is linear in $x = NJ_1^{\nu}$, where the scaling exponent of the energy gap is ν. We should note that in using the Lanczos method we are limited to consider very small sizes ($N_{\max} = 24$). Moreover, since the scaling behavior is restricted to the limit $J_1 \longrightarrow 0$, to find the correct exponent of the energy gap, we should consider very small values of $J_1 < 0.01$. Therefore, using the Lanczos method, the value of scaling variable x cannot be increased into the required amount. However, we are not allowed to read the scaling exponent of the energy gap which exists in the thermodynamic limit ($N \longrightarrow \infty$ or $x \gg 1$). Thus, we have to find the scaling behavior from the small-x regime.

In the following, to find the critical exponent of the energy gap in the small-x region, we apply an applicable method based on perturbation theory [18–20]. In vicinity of the multicritical point, the Hamiltonian can be divided into unperturbed (H_0) and perturbed (H_1) parts as

$$\begin{aligned} \mathcal{H}_0 &= \sum_{j=1}^{N/2} \left(\sigma_{2j-1}^{y}\sigma_{2j}^{y} + \sigma_{2j}^{x}\sigma_{2j+1}^{x}\right)\,, \\ \mathcal{H}_1 &= \sum_{j=1}^{N/2} \left(J_1\sigma_{2j-1}^{x}\sigma_{2j}^{x} - J_1\sigma_{2j-1}^{y}\sigma_{2j}^{y}\right)\,. \end{aligned} \tag{15}$$

In this case, the energy gap basically represents the perturbed behavior

$$G(N, J_1) = B^{(0)}(N) + B^{(1)}(N)J_1 + B^{(2)}(N)J_1^2 + \dots \tag{16}$$

The effect of higher-order terms can be neglected for $J_1 < 0.01$ to a very good approximation. The first coefficient in the perturbation expansion $B_0(N)$ is the same as $G(N, 0)$. To find a relation between other coefficients and correct critical exponent of the gap of energy, it is more convenient to rewrite the energy gap (Eq. (11)) as

$$N\, G(N, J_1) = g\left((N J_1^{\nu})^{\frac{1}{\nu}}\right) , \tag{17}$$

where $f(x) = Ng(x)$. This implies

$$\frac{\partial^m G}{\partial J_1^m}|_{J_1=0} = N^{\frac{m}{\nu}} \times \text{const} , \tag{18}$$

where m is the order of the leading term in the perturbation expansion. Using Eq. (16), we obtain

$$B^{(m)}(N) \propto N^{\frac{m}{\nu}} . \tag{19}$$

Now, by considering the large-N behavior of $B^{(m)}(N)$ as

$$\lim_{N\to\infty} B^{(m)}(N) \simeq a_1 N^{\theta} , \tag{20}$$

we find that the critical exponent of the energy gap is related to the θ-exponent as

$$\nu = \frac{m}{1+\theta} . \tag{21}$$

The above arguments suggest that we should look for the large-N behavior of the coefficient $B^{(m)}(N)$. To do this, in the first step, we plotted in Fig. 1 the energy gap $G(N, J_1)$ *versus* J_1 ($0.001 < J_1 < 0.01$) for a fixed size $N = 24$. The best fit to our data is obtained with $m = 1$. We have also implemented our procedure for different values of sizes $N = 8, 12, 16, 20$ and found the same results for m, as expected. In the second step, we fitted the results of the energy gap $G(N, J_1)$ to the polynomials for values of J_1 close to $J_1 = 0$ up to $m = 1$. Using this procedure, we found the coefficient of the first-order correction perturbation, $B^{(1)}(N)$, as a function of N. Then we plotted in Fig. 2 the function $B^{(1)}(N)$ *versus* N. The results have been plotted for different sizes $N = 8, 12, 16, 20, 24$ to derive the θ-exponent. We

found the best fit data for $\theta = 0.0$. Therefore, using Eq. (21) we have computed the exponent of the energy gap in the vicinity of the multicritical point, $\nu = 1.0 \pm 0.01$ is in complete agreement with the analytical results [5].

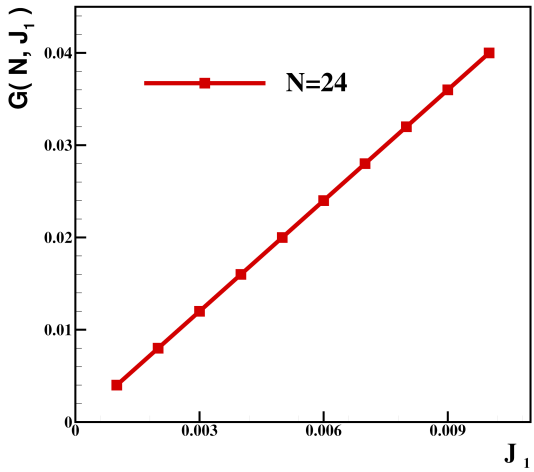


Fig. 1. The energy gap, $G(N, J_1)$ is plotted as a function of J_1 $(0.001 < J_1 < 0.01)$ for the chain size $N = 24$.

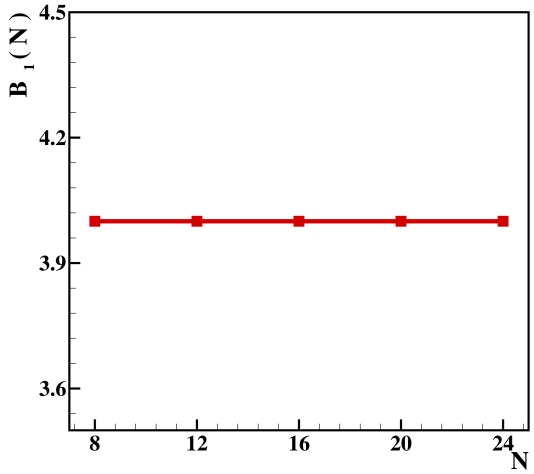


Fig. 2. The values of function $B^{(1)}(N)$ *versus* N. The numerical results are obtained for different sizes $N = 8, 12, 16, 20, 24$.

There is an ambiguity in degeneracy of the ground state of energy [1, 2]. It has been calculated and different results have been obtained. Therefore, to find a better picture of degeneracy, we have calculated energy spectrum

of the model at the multicritical point by using full diagonalization method. Our results show that degeneracy of the ground state energy is $2^{\frac{N}{2}-1}$ and in complete agreement with the results of Brzezicki [1]. Furthermore, we have investigated the degeneracy of the first excited state energy and found it $2^{\frac{N}{2}}$.

4. Conclusion

In this work, we have considered the 1D spin-1/2 quantum compass model. The ground state phase diagram of the model is known very well. It was shown that there is a multicritical point, where the line of the first-order transition ($J_1/L = 0$) meets with a line of the second-order ($J_2/L = 1$) transition. Using the fermionization technique, we have diagonalized the Hamiltonian of the model in the multicritical point. Using the fermion operators, we have found exact expressions for the spin–spin correlation functions in the multicritical point. The results show that the spins on odd (or even) sites are not correlated but otherwise spin–spin correlation functions in the x and y directions are the same and behave as $\langle\sigma^x_{2j-1}\sigma^x_{2j+2n}\rangle = \langle\sigma^y_{2j-1}\sigma^y_{2j+2n}\rangle = -\frac{2}{\pi}[\frac{(-1)^n}{1+2n}]$. We should mention that the correlation function in the z direction is zero.

On the other hand, we have calculated the critical exponent of energy gap in the vicinity of the multicritical point by using the finite size scaling method. Our results show the critical exponent of the energy gap is equal to one $\nu = 1$ and in good agreement with the analytical results. Furthermore, the degeneracy of the ground state and first excited state of energies have been determined by the full diagonalization method, respectively, $2^{\frac{N}{2}-1}$ and $2^{\frac{N}{2}}$.

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