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Emptiness formation probability for the spin-$\frac{1}{2}$ XX chain with three spin and uniform long-range interactions

P.Lou[1,2], J.Y.Lee[1]

[1] Department of Chemistry, Sungkyunkwan University, Suwon 440–746, Korea

[2] Department of Physics, Anhui University, Hefei 230039, Anhui, P.R. China

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The emptiness formation probability (EFP) that the first n spins of the chain are all aligned downwards is studied for the one-dimensional spin-$\frac{1}{2}$ XX chain system with both critical and non-critical regimes with three spin and uniform long-range interactions. By using the emptiness formation probability $P(n)$, the block-block entanglement S_n and the magnetization M^z, the properties of the system are also studied. It is worthy of note that when the quantum phase transition from the phase III to the phase II occurs, the Emptiness Formation Probability $P(n)$ of the system *decreases*, but the block-block entanglement S_n *increases*.

Key words: *emptiness formation probability, spin-$\frac{1}{2}$ XX chain, three spin and uniform long-range interactions*

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1. Introduction

One of the most important issues emerging from the studies of condensed matter physics in recent years is the concept of quantum criticality [1]. A quantum critical point marks a zero-temperature phase transition between different ground states of a many body system as a result of changes in parameters of the underlying Hamiltonian. It was previously stated at the quantum critical point that there is no characteristic length or energy scale, and the system shows power-law spatial correlations and gapless excitations [2]. Moreover, quantum phase transitions can occur between phases that are not characterized by any local order parameter or symmetry breaking description, but that have different quantum order, which is one of the most exciting and novel streams of research in theoretical condensed matter [3].

Recently, quantum phase transitions have been studied in the context of the theory of entanglement where the points of quantum phase transitions are believed to be connected to the points of extremality for the entanglement or its derivatives [4–9]. There are two widely used methods of characterizing entanglement in quantum phase transitions of spin chains. The first method describes the entanglement between two spins in the chain with the quantity called concurrence [10,11]. The other method measures entanglement of a block of spins with the rest of the chain with the von Neumann entropy (block-block entanglement), when the chain is in its ground state [12–17].

Recently we studied the block-block entanglement and quantum phase transition of the system [17], based on the spin-$\frac{1}{2}$ XX chain model with three-spin and uniform long-range interactions [18]. We found that a generic finite order quantum phase transition in the chain can be consistently identified and characterized by studying the behavior of the entanglement of the block with the rest of the chain and its derivatives with respect to the parameter that controls the transition. However, the very important quantity that characterizes a quantum spin system in the quantum spin-liquid phase, which is the so-called EFP [19,20], i.e, the probability to find a ferromagnetic string of the length "n" in the spin liquid ground state, has not been studied for such systems so far. The motivation to study the EFP for this system is to explore if the EFP can supply new important information, just as the block-block entanglement, to gain a deeper understanding of the quantum states of system at zero temperature.

In this paper, we study the probability of the formation of a ferromagnetic string in the ground state of the spin-$\frac{1}{2}$ XX chain model with three-spin and uniform long-range interactions [18]. We show that a generic finite order quantum phase transition in the system can be consistently identified and characterized by studying the EFP behavior and its derivatives with respect to the parameter that controls the transition. In section II, we present the model and theory that we employed. The EFP behavior is studied in section III. In section IV, we give the summary.

2. Model and theory

The exactly solvable quantum spin model considered here is the spin-$\frac{1}{2}$ XX chain with three-spin and uniform long-range interactions, which is defined by the following Hamiltonian [18],

$$H = -\sum_{l=1}^{N}\left[(S_l^x S_{l+1}^x + S_l^y S_{l+1}^y) + \alpha(S_{l-1}^x S_l^z S_{l+1}^y - S_{l-1}^y S_l^z S_{l+1}^x)\right] - \frac{\lambda}{N}\sum_{l,k=1}^{N} S_l^z S_k^z\,, \tag{1}$$

where S_l^i $(i = x, y, z)$ are spin operators of $S = 1/2$ on site l associated with the periodic boundary conditions $(S_{N+1}^i = S_1^i)$, N is the total number of spins, α is the dimensionless parameter characterizing the three-spin coupling constant (in unit of the nearest-neighbor exchange coupling), and λ is the dimensionless parameter characterizing the uniform long-range interactions. This model can be solved by using the Jordan-Wigner transformation [17,18,21,22] and the Hubbard- Stratonovich transformation, and all the physical quantities can be calculated exactly [18]. The ground state energy of the system is given by

$$e_0(\alpha,\lambda) = -\frac{1}{N}\sum_k\left[\cos(k) - \frac{\alpha}{2}\sin(2k)\right]\Theta\left[\epsilon_k(M^z)\right] - \lambda\left(M^z\right)^2, \tag{2}$$

where $\Theta(x) = 1$ when $x > 0$ and vanishes otherwise, and

$$\epsilon_k(M^z) = \cos(k) - \frac{\alpha}{2}\sin(2k) + 2\lambda M^z. \tag{3}$$

The magnetization (M^z) is given by

$$M^z = \frac{1}{N}\sum_k \Theta\left[\epsilon_k(M^z)\right] - \frac{1}{2}\,. \tag{4}$$

Using equations (2), (3), and (4), the magnetization M^z and its contour map can be calculated with parameters λ and α, and the result is shown in figure 1 [17]. It is clearly seen that there

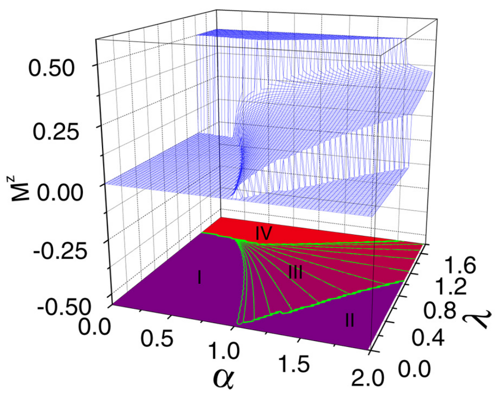

Figure 1. The magnetization M^z and its contour map changes with parameter λ and α.

are four phases. Phases I and II are paramagnetic. But phase II breaks the chiral symmetry [21]. Phases III and IV are ferromagnetic. In phase III (called ferromagnetic δ phase), the magnetic moment $M^z < \frac{1}{2}$, while in phase IV (called ferromagnetic γ), $M^z \equiv \frac{1}{2}$. There are two tricritical points, one separates the paramagnetic, ferromagnetic δ, and paramagnetic chiral phases, and the other separates the paramagnetic, ferromagnetic δ, and ferromagnetic γ phases. The quantum phase transition from phase I to phase IV is of the first order, which results from the uniform long-range interactions. The quantum phase transition from phase III to phase II, as well as from phase IV to phase III, is also of the first order, but it is caused mainly by the three-spin interactions. The quantum phase transition from phase I to phase III is also caused mainly by the three-spin interactions, but it is of the second-order.

The EFP at zero temperature is defined to be the probability of formation of a ferromagnetic string, i.e., the probability that the first n spins of the chain are *all aligned downwards* in the spin liquid ground state $|0\rangle$ [19,20], and it can be expressed as

$$P(n) \quad = \quad \left\langle 0 \left| \prod_{j=1}^{n} \left(S_j^z + \frac{1}{2} \right) \right| 0 \right\rangle \quad . \tag{5}$$

By performing Jordan-Wigner transformation [22],

$$\begin{aligned} S_l^x &= \frac{1}{2} \prod_{j=1}^{l-1} (1 - 2c_j^\dagger c_j)(c_l^\dagger + c_l), \\ S_l^y &= \frac{1}{2i} \prod_{j=1}^{l-1} (c_l^\dagger - c_l)(1 - 2c_j^\dagger c_j), \\ S_l^z &= c_l^\dagger c_l - \frac{1}{2}, \end{aligned} \tag{6}$$

and it is easy to show that equations (5) becomes

$$P(n) = \left\langle 0 \left| \prod_{j=1}^{n} c_j^\dagger c_j \right| 0 \right\rangle = \det \left[\left\langle 0 | c_l^\dagger c_m | 0 \right\rangle \right]_{l,m=1}^{n} , \tag{7}$$

where we have used Wick's theorem. The determinant like equation (7) is referred to as a Toeplitz determinant. Therefore, in our model, the determinant $P(n)$ is

$$P(n) \quad = \quad \begin{vmatrix} f_{1,1} & f_{1,2} & \cdots & f_{1,n} \\ f_{2,1} & f_{2,2} & \cdots & f_{2,n} \\ \cdots & \cdots & \cdots & \cdots \\ f_{n,1} & f_{n,2} & \cdots & f_{n,n} \end{vmatrix} , \tag{8}$$

in which the coefficients $f_{m,n}$ for an infinite chain are calculated by

$$f_{m,n} = \langle 0 | c_m^+ c_n | 0 \rangle = \frac{1}{2\pi} \int \exp(-\mathrm{i}k(n-m)) \mathrm{d}k \Theta(\epsilon_k(M^z)). \tag{9}$$

It is noted that the correlation matrix F_n of the determinant $P(n)$ is

$$F_n \quad = \quad \begin{bmatrix} f_{1,1} & f_{1,2} & \cdots & f_{1,n} \\ f_{2,1} & f_{2,2} & \cdots & f_{2,n} \\ \cdots & \cdots & \cdots & \cdots \\ f_{n,1} & f_{n,2} & \cdots & f_{n,n} \end{bmatrix} , \tag{10}$$

which is the correlation matrix of the reduced density matrix (ρ_L) of n contiguous spins [17]. Then, the von Neumann entropy of a block of n contiguous spins, describing entanglement of the block with the rest of the chain, takes the form [17]

$$S_n = \sum_{j=1}^{n} \left[-(1-\lambda_j)\log_2(1-\lambda_n) - \lambda_j \log_2 \lambda_j \right], \tag{11}$$

where λ_j is the j-th eigenvalue of the correlation matrix F_n. Then, the EFP of the system is given by

$$P(n) = \prod_{j=1}^{n} \lambda_j, \tag{12}$$

i.e, the EFP of the system is the product of the eigenvalues of the correlation matrix F_n.

For example, the entanglement between one spin and the rest part of the system can be characterized by the von Neumann entropy,

$$S_1 = -(\lambda_1)\log(\lambda_1) - (1-\lambda_1)\log(1-\lambda_1), \tag{13}$$

with

$$\lambda_1 = f_{1,1} = \frac{1}{2} + M^z. \tag{14}$$

The EFP of the system is

$$P(1) = \frac{1}{2} + M^z. \tag{15}$$

The entanglement between two contiguous spins and the rest part of the system is characterized by,

$$S_2 = -(\lambda_1)\log(\lambda_1) - (1-\lambda_1)\log(1-\lambda_1) - (\lambda_2)\log(\lambda_2) - (1-\lambda_2)\log(1-\lambda_2), \tag{16}$$

in which

$$\begin{aligned} \lambda_1 &= f_{1,1} - f_{1,2} = \frac{1}{2} + M^z - f_{1,2}, \\ \lambda_2 &= f_{1,1} + f_{1,2} = \frac{1}{2} + M^z + f_{1,2}. \end{aligned} \tag{17}$$

Then, the EFP of the system is

$$P(2) = \left(\frac{1}{2} + M^z\right)^2 - (f_{1,2})^2. \tag{18}$$

It is important to note that both the EFP and block-block entanglement of the system are directly related to the eigenvalues of the correlation matrix F_n. Therefore, one can expect that the quantum phase transitions of the system can be well identified by the EFP $P(n)$, just like the block-block entanglement [17].

3. Results and discussion

We first investigate the $\lambda = 0$ case. In this case, there are two phases in the system. The ground state of the new phase is a chiral state $O_k > 0$ with gapless excitations [21]. It is separated by the critical point $\alpha_c = 1$ from the ground state of $O_k = 0$ gapless phase. For the two phases, $M^z = 0$ and

$$f_{l,l+m} = \begin{cases} \dfrac{1}{m\pi}\sin\left(m\dfrac{\pi}{2}\right), & \alpha < 1, \\ \dfrac{1}{2m\pi}\left[1-(-1)^m\right]\sin\left(m \arcsin\left(\dfrac{1}{\alpha}\right)\right), & \alpha \geqslant 1, \end{cases} \tag{19}$$

and

$$f_{l,l} = \frac{1}{2}, \tag{20}$$

for all α. Then, the results of S_1, S_2, S_3 and S_4 are given as follows, respectively [17].

$$S_1 = 1, \tag{21}$$

$$S_2 = \begin{cases} 2 - \left[(1-\frac{2}{\pi})\log_2(1-\frac{2}{\pi}) + (1+\frac{2}{\pi})\log_2(1+\frac{2}{\pi})\right], & \alpha < 1, \\ 2 - \left[(1-\frac{2}{\pi\alpha})\log_2(1-\frac{2}{\pi\alpha}) + (1+\frac{2}{\pi\alpha})\log_2(1+\frac{2}{\pi\alpha})\right], & \alpha \geqslant 1, \end{cases} \tag{22}$$

and

$$S_3 = \begin{cases} 3 - \left(1-\frac{2\sqrt{2}}{\pi}\right)\log_2\left(1-\frac{2\sqrt{2}}{\pi}\right) - \left(1+\frac{2\sqrt{2}}{\pi}\right)\log_2\left(1+\frac{2\sqrt{2}}{\pi}\right), & \alpha < 1, \\ 3 - \left(1-\frac{2\sqrt{2}}{\pi\alpha}\right)\log_2\left(1-\frac{2\sqrt{2}}{\pi\alpha}\right) - \left(1+\frac{2\sqrt{2}}{\pi\alpha}\right)\log_2\left(1+\frac{2\sqrt{2}}{\pi\alpha}\right), & \alpha \geqslant 1. \end{cases} \tag{23}$$

It is noted that $\mathrm{d}S_1/\mathrm{d}\alpha = 0$, but

$$\frac{\mathrm{d}S_2}{\mathrm{d}\alpha} = \begin{cases} 0, & \alpha < 1, \\ \frac{2}{\pi\alpha^2}\log_2\left(\frac{1+\frac{2}{\pi\alpha}}{1-\frac{2}{\pi\alpha}}\right), & \alpha \geqslant 1, \end{cases} \tag{24}$$

and

$$\frac{\mathrm{d}S_3}{\mathrm{d}\alpha} = \begin{cases} 0, & \alpha < 1, \\ \frac{2\sqrt{2}}{\pi\alpha^2}\log_2\left(\frac{1+\frac{2\sqrt{2}}{\pi\alpha}}{1-\frac{2\sqrt{2}}{\pi\alpha}}\right), & \alpha \geqslant 1. \end{cases} \tag{25}$$

While, the EFP of the system are

$$P(1) = \frac{1}{2}, \tag{26}$$

$$P(2) = \begin{cases} \frac{1}{4} - \left(\frac{1}{\pi}\right)^2, & \alpha < 1, \\ \frac{1}{4} - \left(\frac{1}{\pi}\right)^2\left(\frac{1}{\alpha}\right)^2, & \alpha \geqslant 1, \end{cases} \tag{27}$$

and

$$P(3) = \begin{cases} \frac{1}{8} - \left(\frac{1}{\pi}\right)^2, & \alpha < 1, \\ \frac{1}{8} - \left(\frac{1}{\pi}\right)^2\left(\frac{1}{\alpha}\right)^2, & \alpha \geqslant 1. \end{cases} \tag{28}$$

It is also noted that $\mathrm{d}P(1)/\mathrm{d}\alpha = 0$, but

$$\frac{\mathrm{d}P(2)}{\mathrm{d}\alpha} = \begin{cases} 0, & \alpha < 1, \\ 2(\frac{1}{\pi})^2(\frac{1}{\alpha})^3, & \alpha \geqslant 1, \end{cases} \tag{29}$$

and

$$\frac{\mathrm{d}P(3)}{\mathrm{d}\alpha} = \begin{cases} 0, & \alpha < 1, \\ 2(\frac{1}{\pi})^2(\frac{1}{\alpha})^3, & \alpha \geqslant 1. \end{cases} \tag{30}$$

It is displayed that at $\alpha_c = 1$, the behavior of EFP $P(n)$ is similar to that of the block-block entanglement S_n, i.e, the first derivative of the EFP, $\mathrm{d}P(n)/\mathrm{d}\alpha$ shows discontinuities, while $P(n)$ is continuous. The discontinuity in $\mathrm{d}P(n)/\mathrm{d}\alpha$ at $\alpha_c = 1$ does indicate the second-order quantum phase transitions of the present case. Thus, there is one-to-one correspondence between quantum phase transitions and the non-analyticity property of the EFP $P(n)$.

When $\alpha \to \infty$, from the equation (19) we get

$$f_{l,l+m} = f_{l+m,l} = 0, \tag{31}$$

for $m \geqslant 1$. Thus

$$P(n) = \left(\frac{1}{2}\right)^n . \tag{32}$$

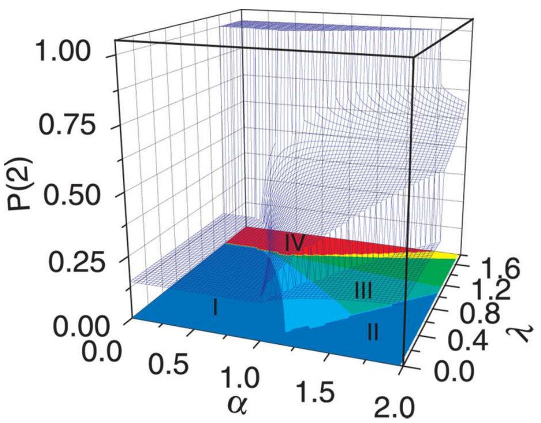

Figure 2. The Emptiness Formation Probability $P(n)$ and its contour map changes with parameter λ and α for $n = 2$.

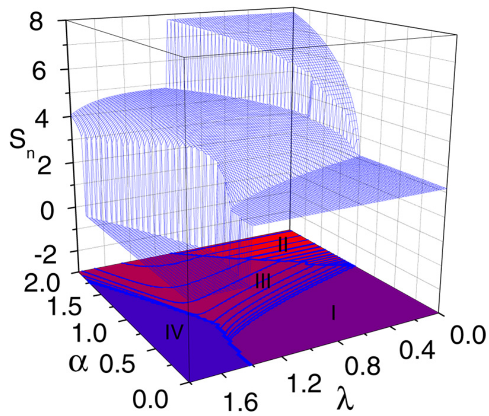

Figure 3. The block-block entanglement S_n and its contour map changes with parameter λ and α for $n = 10$.

The numerical results for the EFP $P(n)$ and its contour map with the variation of the parameters λ and α for $n = 2$ are displayed in figure 2. The numerical results for the block-block entanglement S_n and its contour map changes with parameters λ and α for $n = 10$ are displayed in figure 3. Comparing figure 2 with figure 1 and figure 3, it is noted that the phase diagrams are consistent with each other. This means that there is one-to-one correspondence between quantum phase transitions and the non-analyticity property of the EFP $P(n)$ for the present model as well.

We have farther studied the properties of phases I, II, III and IV by using the combination of the EFP $P(n)$, the block-block entanglement S_n, and the magnetization M^z. Firstly, from the magnetization M^z aspect angle, phases I and II are *paramagnetic*. Phases III and IV are *ferromagnetic phases*. The M^z value is zero in both phases I and II. But, there is difference in between phases III and IV. In phase III (called ferromagnetic δ phase), the magnetic moment $M^z < \frac{1}{2}$, while in phase IV (called ferromagnetic γ), $M^z \equiv \frac{1}{2}$ in the long-range ordered *ferromagnetic phase*. Thus, the magnetization M^z can be used to identify phases III and IV, but cannot be used to characterize phases I and II. Secondly, the block-block entanglement S_n can be used to identify phases I, II, III and IV, which may be seen from figure 3. The EFP $P(n)$, just as the block-block entanglement S_n, can also be used to distinguish the different phases of system as shown in figure 2. For example, when the system is in the phase IV, since $M^z \equiv \frac{1}{2}$, and we have

$$f_{l,l} \quad = \quad 1, \tag{33}$$

and

$$f_{l,l+m} = f_{l+m,l} = 0. \tag{34}$$

Thus

$$P(n) \quad = \quad 1. \tag{35}$$

This implies that the probability to find a ferromagnetic string of the length "n" in the ground state of phase IV is always 1, i.e, the long-range ordered *ferromagnetic phase*. While

$$S_n \quad = \quad 0. \tag{36}$$

This indicates that the ground state of phase IV is ordered phase, and has no entanglement and spin fluctuation.

It is noted that the behavior of the system occurs in between the phase II and III. If the quantum phase transition takes place from the phase III to phase II, the EFP of the system *decreases*, but the block-block entanglement S_n *increases*. That is to say, the phase III is *more ordered*(short-range ordered), while the phase II is *more entangled*, and more *spin fluctuating* due to the *quantum frustration* of the system.

4. Summary

In summary, we have explored the Emptiness Formation Probability $P(n)$, the block-block entanglement S_n, the magnetization M^z, and quantum phase transition, based on an exactly solvable model of the spin-$\frac{1}{2}$ XX Heisenberg chain with three-spin and uniform long-range interactions. We find that the quantum phase transition is well characterized, just as the block-block entanglement [17], by the Emptiness Formation Probability of the system. The evolution of the system shows a number of characteristic features in the Emptiness Formation Probability $P(n)$, the block-block entanglement S_n, and the magnetization M^z. The EFP extends and deepens our previous understanding of quantum phase transitions.

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References

1. Sachdev S., Quantum Phase Transitions. Cambridge University Press, Cambridge, 1999.
2. Pachos J. K., Carollo A. C. M., Phil. Trans. R. Soc. A, 2006, **364**, 3463.
3. Wen X-G., Quantum Field Theory of Many-Body Systems. Oxford University Press, 2004.
4. Chen Y., Zanardi P., Wang Z.D., Zhang F.C., New Journal of Physics, 2006, **8**, 97.
5. Gu S.-J., Tian G.-S., Lin H.-Q., New Journal of Physics, 2006, **8**, 61.
6. Wu L.-A., Sarandy M.S., Lidar D. A., Phys. Rev. Lett, 2004, **93**, 250404.
7. Latorre J.I., Rico E., Vidal G., Quantum Inf. Comput, 2004, **4**, 48.
8. Yang M.-F., Phys. Rev. A, 2005, **71**, 030302(R).
9. Gu S.-J., Deng S.-S., Li Y.-Q., Lin H.-Q., Phys. Rev. Lett, 2004, **93**, 86402.
10. Osterloh A., Amico L., Falci G., Fazio R., Nature (London), 2002, **416**, 608.

11. Osborne T. J., Nielsen M. A., Phys. Rev. A, 2002, **66**, 032110.
12. Vidal G., Latorre J. I., Rico E., Kitaev A., Phys. Rev. Lett, 2003, **90**, 227902.
13. Jin B. Q., Korepin V. E., J. Stat. Phys, 2004, **116**, 79.
14. Fannes M., Haegemann B., Mosonyi M., J. Math. Phys, 2003, **44**, 6005.
15. Keating J. P., Mezzadri F., Commun. Math. Phys, 2004, **252**, 543.
16. Popkov V., Salerno M., Phys. Rev. A, 2005, **71**, 012301.
17. Lou P., Lee J. Y., Phys. Rev. B, 2006, **74**, 134402.
18. Lou P., Phys. Rev. B, 2005, **72**, 064435.
19. Korepin V. E., Izergin A. G., Essler F. H. L., Uglov D. B., Phys. Lett. A, 1994, **190**, 182.
20. Franchini F., Abanov A.G., J. Phys. A, 2005, **38**, 5069.
21. Lou P., Wu W.-C., Chang M.-C., Phys. Rev. B, 2004, **70**, 064405.
22. Jordan P., Wigner E., Z. Physik, 1928, **47**, 631.

Ймовірність формування порожнини для спін-$\frac{1}{2}$XX ланцюжка з триспіновою та однорідною далекосяжною взаємодіями

П.Лу[1,2], Ж.Й.Лі[2]

[1] Факультет хімії, Університет Сунгкянкван, Сувон, Корея

[2] Факультет фізики, університет Ангуі, Гефей Ангуі, Китайська Народна Республіка

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Досліджується ймовірність формування порожнини, тобто ймовірність того, що n перших спінів у ланцюжку є спрямовані вниз, для одновимірної спін-$\frac{1}{2}$XX ланцюжкової системи з триспіновою і однорідною далекосяжною взаємодіями як у критичному, так і у некритичному режимах. З використанням ймовірності формування порожнини $P(n)$, блок-блок сплутаності S_n і намагніченості M^z досліджуються також властивості такої спінової системи. Важливо відзначити, що коли відбувається квантовий фазовий перехід з фази III у фазу II, ймовірність формування порожнини системи $P(n)$ зменшується, тоді як блок-блок сплутаність S_n зростає.

Ключові слова: *ймовірність формування порожнини, спін-$\frac{1}{2}$XX ланцюжок, триспінові і однорідні далекосяжні взаємодії*

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