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2005 J. Phys. A: Math. Gen. 38 7377

(http://iopscience.iop.org/0305-4470/38/33/011)

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS A: MATHEMATICAL AND GENERAL

J. Phys. A: Math. Gen. **38** (2005) 7377–7388 doi:10.1088/0305-4470/38/33/011

Entanglement of periodic anisotropic XY chains

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Received 28 January 2005, in final form 27 June 2005
Published 3 August 2005
Online at stacks.iop.org/JPhysA/38/7377

Abstract

By using the concept of concurrence, the entanglement of periodic anisotropic XY chains in a transverse field is studied numerically. It is found that the derivatives $\partial_\lambda C(1)$ of nearest-neighbour concurrence diverge at quantum critical points. By proper scaling, we found that all the derivatives $\partial_\lambda C(1)$ for periodic XY chains in the vicinity of quantum critical points have the same behaviours as that of a uniform chain.

PACS numbers: 03.65.Ud, 02.30.Ik, 05.50.+q

1. Introduction

Quantum entanglement is the most remarkable trait of quantum systems and cannot be accounted for classically. The early study of entanglement is only focused on the foundations of quantum mechanics [1]. Recently, due to its potential applications in quantum communications, quantum cryptography, quantum computer and quantum information [2], entanglement has been studied extensively. One of the most important progresses is the quantitative measures of entanglement for the *mixed* state by using the *entanglement of formation* [3, 4]. For the special case of two spin-$\frac{1}{2}$ systems, the entanglement of formation is given by the concurrence C [5, 6].

On the other hand, there has been much interest in the quantum phase transition recently [7]. Usually, the quantum phase transitions are associated with the changes of the ground-state wavefunction. Therefore, it is natural to see if there are changes in the entanglement at the quantum phase transition point. Recently, there were some works [8–11] on the relationship between the entanglement and the quantum phase transition of the spin chains. By using the concurrence, Osterloh *et al* [9] found that there is a universal scaling behaviour for the derivatives of the entanglement of the uniform anisotropic XY chain in the vicinity of the quantum phase transition. The von Neumann entropy of a large block of neighbouring spins

and its singularity at the quantum phase transition point have been studied for XXZ [10, 11] and XY spin chains [10, 12].

Recently, we studied the quantum phase transitions of periodic and quasiperiodic anisotropic XY chains in a transverse field and found that there are more than one quantum phase transition point (QPTP) on some parameter regions for periodic and quasiperiodic chains, and the number of QPTPs is dependent on the parameters and the structure of systems, which is quite different from those of the quantum Ising chain in a transverse field and the uniform anisotropic XY chain without transverse field [13]. In this paper, we shall study the behaviour of the entanglement in the vicinity of quantum phase transition of periodic anisotropic XY model by using the concept of concurrence.

The paper is organized as follows. In section 2, we introduce the formula and method with which we can study the entanglement of the periodic anisotropic XY chain. In section 3, we discuss the finite-size effect and boundary condition for the spin chain. In section 4, we study the behaviour of the entanglement of the periodic chains by numerical results. We present some discussions and conclusions in section 5.

2. Formula and method

The Hamiltonian of the general anisotropic XY model in a transverse field is given by

$$H = -\sum_{i=1}^{N}\left\{\frac{\lambda_i}{2}\left[(1+\gamma)\sigma_i^x\sigma_{i+1}^x + (1-\gamma)\sigma_i^y\sigma_{i+1}^y\right] + \sigma_i^z\right\}, \tag{1}$$

where λ_i are the nearest-neighbour interactions, σ_i^α the αth Pauli matrix ($\alpha = x$, y or z) on site i, N the number of sites, and γ the degree of anisotropy. For $\lambda_i = \lambda$, the model is a uniform quantum spin chain. For the model of a period-two quantum spin chain, $\lambda_{2i} = \lambda$, $\lambda_{2i+1} = \beta\lambda$.

By use of the famous Jordan–Wigner transformation, the Hamiltonian can be written as

$$H = -\sum_{j=1}^{N}\left\{-\lambda_j\left(c_j^+c_{j+1} + c_{j+1}^+c_j\right) - 2c_j^+c_j + \left[-\frac{\lambda_j\gamma}{2}\left(c_j^+c_{j+1}^+ - c_{j+1}^+c_j^+\right) + \text{h.c.}\right]\right\} + N$$
$$+\left[\lambda_N\left(c_N^+c_1 - c_Nc_1^+\right) + \lambda_N\gamma\left(c_N^+c_1^+ - c_Nc_1\right)\right][\exp(\mathrm{i}\pi\Omega) + 1], \tag{2}$$

where

$$\Omega \equiv \sum_{1}^{N} c_i^+c_i = \sum_{1}^{N}\left(S_i^z + \frac{1}{2}\right), \qquad S_i^z = \frac{1}{2}\sigma_i^z.$$

With neglect of the last term, the Hamiltonian equation (2) can be written as

$$H = -\sum_{i,j=1}^{N}\left[c_i^+A_{ij}c_j + \frac{1}{2}\left(c_i^+B_{ij}c_j^+ + \text{h.c.}\right)\right] + N, \tag{3}$$

where $A_{ij} = -\lambda_i\delta_{j,i+1} - \lambda_j\delta_{j,i-1} - 2\delta_{ij}$, $B_{ij} = -\lambda_i\gamma\delta_{j,i+1} + \lambda_j\gamma\delta_{j,i-1}$; $A_{1N} = -\lambda_N = A_{N1}$, $B_{1N} = -\lambda_N\gamma = -B_{N1}$. The quadratic Hamiltonian equation (2) may be diagonalized by Bogliubov transformation,

$$\eta_k = -\sum_{i=1}^{N}\left(p_{ki}c_i + q_{ki}c_i^+\right), \tag{4}$$

$$\eta_k^+ = -\sum_{i=1}^{N}\left(p_{ki}c_i^+ + q_{ki}c_i\right), \tag{5}$$

where $k = -\frac{N}{2}, -\frac{N}{2}+1, \ldots, \frac{N}{2}-1$; and p_{ki} and q_{ki} can be chosen to be real. By requiring that the operator η_k obey fermionic anticommutation relations, and that the Hamiltonian equation (2) be manifestly diagonal, the following two coupled matrix equations must hold

$$(A-B)\overrightarrow{\phi_k} = \Lambda_k \overrightarrow{\psi_k} \tag{6}$$

$$(A+B)\overrightarrow{\psi_k} = \Lambda_k \overrightarrow{\phi_k}, \tag{7}$$

where $\overrightarrow{\phi_k}, \overrightarrow{\psi_k}$ are two column vectors, and are given by

$$\overrightarrow{\phi_k} = p_{ki} + q_{ki} \tag{8}$$

$$\overrightarrow{\psi_k} = p_{ki} - q_{ki}. \tag{9}$$

Then the Hamiltonian takes the form

$$H = \sum_k \Lambda_k \left(\eta_k^+ \eta_k - \frac{1}{2}\right). \tag{10}$$

Following the study of the uniform anisotropic XY chain [9], we use the concurrence as the measure of the entanglement of two spins in the chain. The concurrence of two spins at sites i and j is defined as

$$C = \max\{0, r_1 - r_2 - r_3 - r_4\}. \tag{11}$$

Here, r_α are the square roots of the eigenvalues of the product matrix $R = \rho_{ij}\widetilde{\rho}_{ij}$ in descending order; the spin flipped matrix $\widetilde{\rho}_{ij}$ is defined as $\widetilde{\rho}_{ij} = (\sigma^y \otimes \sigma^y)\rho_{ij}^*(\sigma^y \otimes \sigma^y)$. The ρ_{ij} is the reduced density matrix and can be written as following operator expansion form [8]

$$\rho_{ij} = \frac{1}{4}\sum_{\alpha,\beta=0}^{3} p_{\alpha\beta}\sigma_i^\alpha \otimes \sigma_j^\beta. \tag{12}$$

The coefficients are determined by the relations

$$p_{\alpha\beta} = \mathrm{tr}\left(\sigma_i^\alpha \sigma_j^\beta \rho_{ij}\right) = \left\langle \sigma_i^\alpha \sigma_j^\beta \right\rangle \tag{13}$$

where $\sigma_i^0 = I$ is the unit matrix of 2×2.

Because of the reflection symmetry, and the global phase flip symmetry, and the Hamiltonian being real, the only nonzero coefficients in equation (12) are $p_{00}, p_{03}, p_{30}, p_{11}, p_{22}, p_{33}$. Furthermore, $p_{00} = 1$, because the density matrix must have trace unity [8]. And the two-point correlation functions are given by [14]

$$\left\langle \sigma_i^x \sigma_j^x \right\rangle = \begin{vmatrix} G_{i,i+1} & G_{i,i+2} & \ldots & G_{ij} \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ G_{j-1,i+1} & G_{j-1,i} & \ldots & G_{j-1,j} \end{vmatrix} \tag{14}$$

$$\left\langle \sigma_i^y \sigma_j^y \right\rangle = \begin{vmatrix} G_{i+1,i} & G_{i+1,i+1} & \ldots & G_{i+1,j-1} \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ G_{j,i} & G_{j,i+1} & \ldots & G_{j,j-1} \end{vmatrix} \tag{15}$$

$$\left\langle \sigma_i^z \sigma_j^z \right\rangle = G_{ii}G_{jj} - G_{ij}G_{ji} \tag{16}$$

$$\left\langle \sigma_i^z \right\rangle = \frac{1}{N}\sum_k G_{ii} \tag{17}$$

where $G_{ij} = -\sum_k \psi_{ki}\phi_{kj}$.

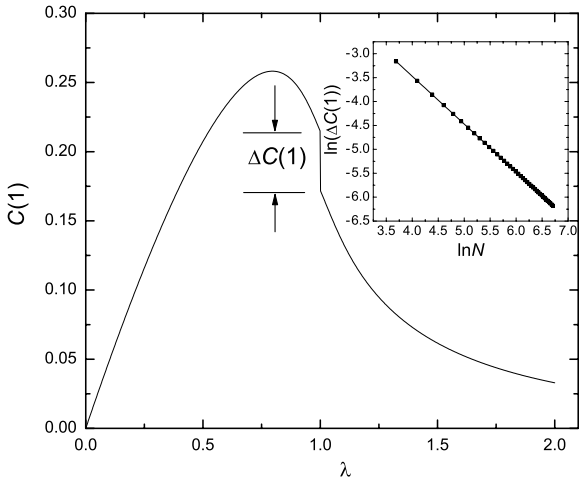

Figure 1. The NNC as a function of λ for the spin chain with $\gamma = 1$ and $N = 40$. There is a gap for the concurrence at quantum phase transition point $\lambda = \lambda_c = 1$. The inset is the gap as a function of number of spins. When $N \to \infty$, the gap tends to N^{-1}.

3. Finite-size effect and boundary terms

For the uniform anisotropic XY chain, Osterloh *et al* [9] found that the derivatives of nearest-neighbour concurrence (NNC) have logarithmic singularities at the QPTPs. But their numerical results are obtained only for chains with odd spins. For the even-spin chains, by using the same method as that of paper [9], we find that there is a gap in the curve of NNC versus λ at quantum phase transition point λ_c (see figure 1). When the number of spins goes to infinite, the gap tends to zero as $\Delta C \sim N^{-1}$ (see the inset of figure 1). Therefore, we can conclude that the gap is caused by the finite-size effect.

The reason for the difference of NNC between the odd and even cases is neglect of the last term of equation (2) in solving the eigenvalues and eigenvectors of the Hamiltonian. The term is proportional to $\exp(\mathrm{i}\pi\Omega)+1$ and only depends on the boundary spins, which has the effect of making changes of the order $1/N$ in k, ϕ_k and ψ_k, all of which are negligible in the calculation of real physical quantities for large system. But the entanglement is a property of ground-state wavefunction and is sensitive to the boundary terms, therefore the last term cannot be neglected. The term depends on the evenness or oddness of Ω, i.e., if $\Omega =$ odd, the term is equal to zero; if $\Omega =$ even, then $\exp(\mathrm{i}\pi\Omega) + 1 = 2$. From the definition of Ω, we can assume that Ω has the same evenness or oddness as that of the size of the spin chain. Consequently when the size of the spin chain is even, the Ω is even, and then the term cannot be neglected for finite-size chain. For even-spin chain the Hamiltonian must be rewritten and the elements of matrix A and B in equation (3) are changed as

$$\begin{aligned} A'_{ij} &= A_{ij}, & B'_{ij} &= B_{ij}, \\ A'_{1N} &= -A_{1N} = \lambda_N = A'_{N1}, & B'_{1N} &= -B_{1N} = -\lambda_N\gamma = -B'_{N1}. \end{aligned} \tag{18}$$

That is, the boundary term is anti-periodic.

In order to test our assumption, we study the NNC of the three-spin and four-spin cases. For these systems, we can obtain the concurrence by solving the Hamiltonian directly.

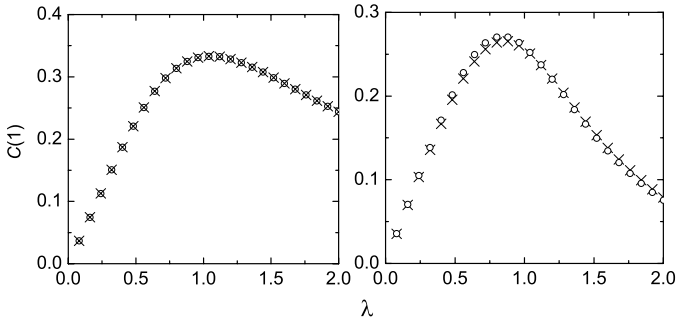

Figure 2. The NNC of three-spin and four-spin chains. The figure on left-hand side is a three-spin case, and the figure on right-hand side is a four-spin case. The results by solving the Hamiltonian directly correspond to the crosses. The circles correspond to the results by Jordan–Wigner transformation, in which we use periodic boundary terms for the three-spin case and anti-periodic boundary terms for the four-spin case.

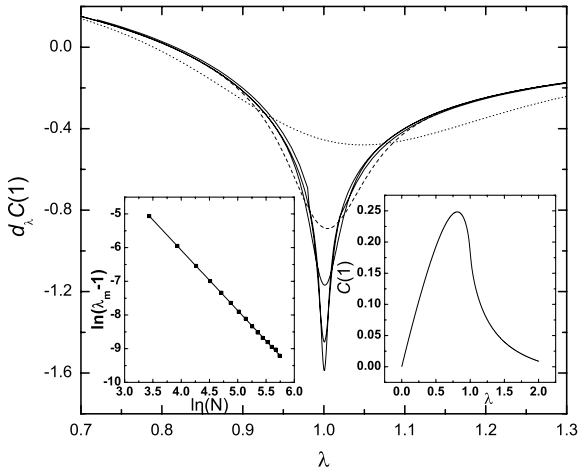

Figure 3. The derivative of NNC $\partial_\lambda C(1)$ as a function of λ for the uniform chain with the anti-periodic boundary terms. The curves correspond to different lattice sizes $N = 10, 40, 100, 250, 400, \ldots$, respectively. On increasing the system size, the minimum changes and tends as $N^{-1.793\,35}$ (left inset) towards the critical point $\lambda_c = 1$. The right inset shows the behaviour of NNC $C(1)$ itself for $N = 100$. The maximum that occurs below λ_c is not related to the critical point, where $\gamma = 0.9$.

The results are the same with those obtaining by solving equation (3) with (anti)periodic boundary for (four-) three-spin system (see figure 2).

Furthermore, we calculate the NNC of the even-spin chains and found that they are the same with the results of the foregone odd-spin chains obtained by Osterloh *et al* [9] (see figure 3). In this figure, we will see that the gap disappears at the critical point, and the minimum of $\partial_\lambda C(1)$ behaves as the odd-spin chains. And the finite-size scaling is the same with the results of odd-spin chains.

Therefore we should use the anti-periodic boundary terms (18) to study the even-spin chains in the following study.

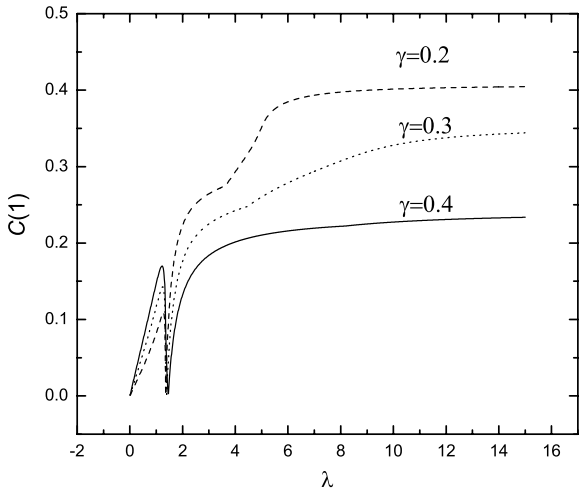

Figure 4. The NNC of the period-two XY chain. In this case we choose $N = 120$, and from the upper curve down to the lower curve on the right, the curves correspond to $\gamma = 0.2, 0.3, 0.4$, respectively. For $\beta = 0.5$, $\gamma_c = \frac{1}{3}$.

4. Entanglement of the periodic spin chains

4.1. The period-two chains

For the periodic-two anisotropic XY chain in a transverse field, $\lambda_{2i} = \lambda$, $\lambda_{2i+1} = \beta\lambda$, it was found [13] that there exists a critical value $\gamma_c = \frac{1-\beta}{1+\beta}$, which is a function of β. For any γ $(0 < \gamma < 1)$, there is a QPTP, and for $\gamma < \gamma_c$ there is an additional QPTP. The QPTPs are

$$\lambda_{C_1} = \frac{2}{\sqrt{(1+\beta)^2 - \gamma^2(1-\beta)^2}}, \qquad \text{for} \quad 0 < \gamma, \quad \beta < 1,$$

$$\lambda_{C_2} = \frac{2}{\sqrt{(1-\beta)^2 - \gamma^2(1+\beta)^2}}, \qquad \text{for} \quad \gamma < \frac{1-\beta}{1+\beta}.$$

This is due to the competition of periodicity and anisotropy. The additional QPTP is the result of two-spin clusters. In the numerical study, for finite-size system the additional QPTP disappears for odd-spin chains. Therefore, we only study even-spin period-two chains. For the period-two chain, the σ_{2i} and σ_{2i+1} are not equivalent, therefore, the nearest-neighbour concurrence $C_{2i,2i+1}$ and $C_{2i+1,2i+2}$ are different. But, they have the similar behaviours with changing of the parameters λ and γ. So that, we use the average concurrence $C = \frac{1}{2}(C_{2i,2i+1} + C_{2i+1,2i+2})$ to study the entanglement. Similarly, we use $C = \frac{1}{3}(C_{3i,3i+1} + C_{3i+1,3i+2} + C_{3i+2,3i+3})$ to study the entanglement of the period-three chains. Figure 4 gives the numerical results of the concurrence for different γ at $\beta = 0.5$. Figure 5 shows the derivative of the concurrence at the vicinity of the QPTPs. From figure 5 we can clearly see that for any γ, there is one QPTP λ_{C_1} (see the figure on the left-hand side), and for $\gamma = 0.2, 0.3 < \gamma_C$ ($\gamma_C = \frac{1}{3}$ for $\beta = 0.5$) there is an additional QPTP while there is none for $\gamma = 0.4$ (see the figure on the right-hand side).

In order to study the behaviour of NNC at the vicinity of QPTPs, we study the derivatives of NNC for different sizes, and found that they have the same behaviour as that of the uniform case. Figure 6 shows the curve of the derivative of the NNC in the neighbourhood of λ_{C_1} the critical point for even-spin chains with a different size. From the figure, we clearly see that

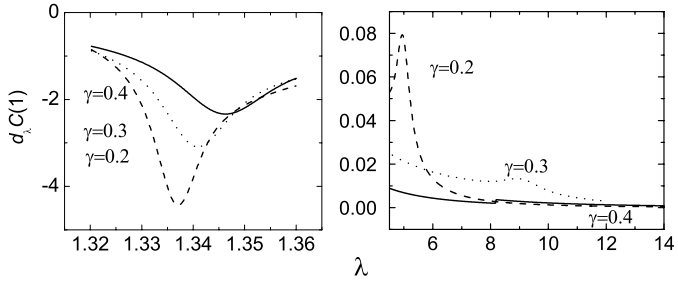

Figure 5. The derivative of the NNC of the period-two XY chain. In this case we choose $N = 120$, and $\gamma = 0.2, 0.3, 0.4$, respectively. The left- and right-hand side figures correspond to the vicinity of λ_{C_1} and λ_{C_2}, respectively.

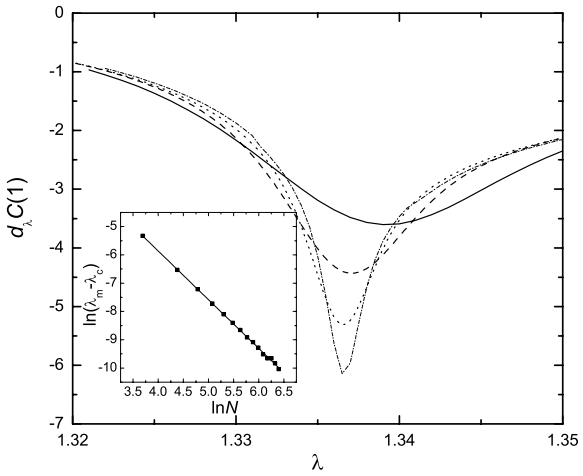

Figure 6. The derivative of the NNC at the vicinity of λ_{C_1}. On increasing the system size, the position of the minimum λ_m changes and tends as $N^{-1.720\,29}$, where $N = 60, 120, 240, 480$, respectively.

the derivative exhibits the same behaviour as that of the uniform chain at the quantum critical point. The minimum λ_m of the curve changes as the increasing system size (see the inset of figure 6), and tends as

$$\lambda_m - \lambda_{C_1} \sim N^{\alpha},$$

where α depends on γ, and $\alpha = -1.72$ for $\gamma = 0.2$. The value $\partial_\lambda C(1)$ at the first point λ_m logarithmically diverges with increasing system size as

$$\partial_\lambda C(1)|_{\lambda_m} = -1.24509 \ln N + \text{const},$$

which can clearly be shown in the inset of figure 7. By proper s scaling [15], it is possible to make all the data of the derivative of NNC for different N collapse approximately onto a single curve with critical exponent $\nu = 1$ (see figure 7 and its caption). For the additional QPTP λ_{C_2} we also use the same method to the NNC and its derivatives. We find that the NNC at the additional QPTP has the similar behaviour as that of at the QPTP λ_{C_1}. The minimum λ_m at the vicinity of the additional QPTP of the curve changes as the increasing system size (the inset of figure 8), and tends as

$$\lambda_m - \lambda_c \sim N^{-1.78712}.$$

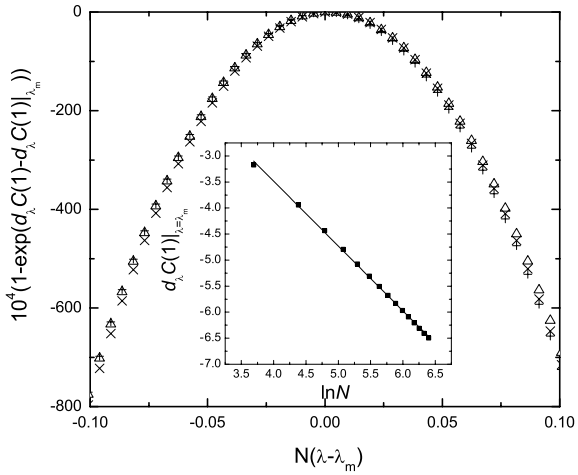

Figure 7. The finite-size scaling is performed for the case of logarithmatic divergence at the vicinity of λ_{C_1} for the period-two chain. The concurrence, considered as a function of the system size and the coupling constant, is a function of $N^{1/\nu}(\lambda - \lambda_{\rm m})$ only. All the data from $N = 240$ up to $N = 1000$ collapse onto a single curve. The critical exponent is $\nu = 1$. The inset shows the divergence of the value at the minimum as the system size increases, where $\gamma = 0.2$

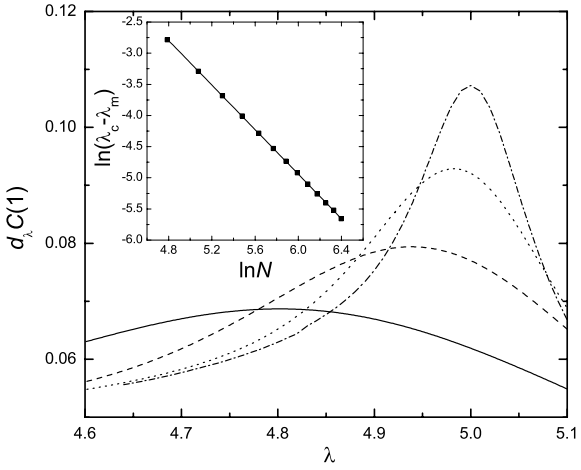

Figure 8. The derivative of the NNC at the vicinity of λ_{C_2}. On increasing the system size, the position of the minimum $\lambda_{\rm m}$ changes and tends as $N^{-1.78712}$, where $N = 60, 120, 240, 480$, from dowm to up, respectively.

The value $\partial_\lambda C(1)$ at the second point $\lambda_{\rm m}$ logarithmically diverges with increasing system size as

$$\partial_\lambda C(1)|_{\lambda_{\rm m}} = 0.02048 \ln N + \text{const},$$

which can clearly be shown in the inset of figure 9. Taking into account the distance of the minimum of $\partial_\lambda C(1)$ of the period-two chain from the additional QPTP, it is possible to make all the data for different N collapse approximately onto a single curve (figure 9), and the critical exponent also is $\nu = 1$.

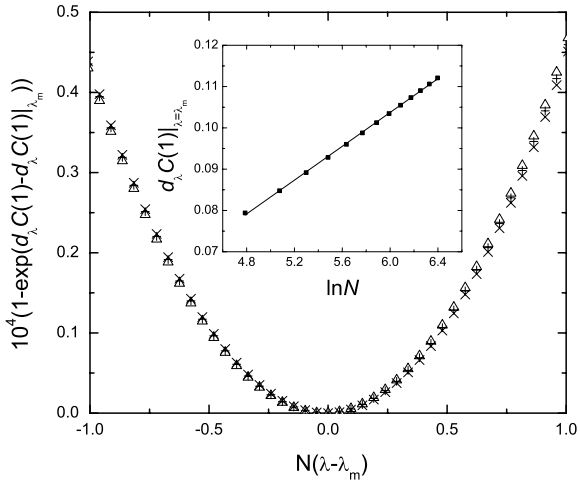

Figure 9. The finite-size scaling is performed for the case of logarithmatic divergence at the vicinity of λ_{C_2} for the period-two chain. All the data from $N = 240$ up to $N = 1000$ collapse onto a single curve. The inset shows the divergence of the value at the minimum as the system size increases, where $\gamma = 0.2$.

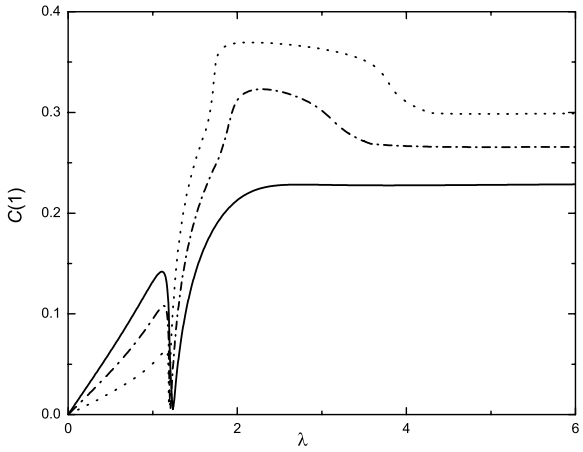

Figure 10. The NNC of the period-three XY chain. In this case we choose $N = 120$, the dotted, dotted-dashed and solid lines correspond to $\gamma = 0.1, 0.2, 0.3$, respectively.

From the above discussion, we can see that the behaviours of the entanglement at the vicinity of both two critical points for the period-two XY chain are similar as that of uniform chain, and belong to the same universality class.

4.2. The period-three chains

For the period-three anisotropic XY spin chain, we choose $\lambda_{3i} = \lambda_{3i+1} = \lambda$, $\lambda_{3i+2} = \beta\lambda$. As same as that of period-two case, it is found that there exists a critical value of γ_c, which is a function of β. For any $0 < \gamma < 1$, there is a QPTP, and for $\gamma < \gamma_c$ there are two additional QPTPs [13]. This is also due to the three-spin cluster. By the same method as that in section 4.1, we calculate the concurrence of the period-three XY chain, from which we can study the behaviour of the entanglement of this case. Figures 10 and 11 give the typical

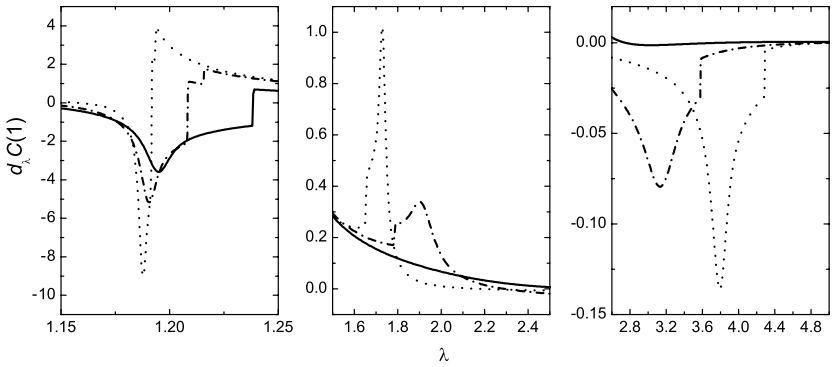

Figure 11. The derivative of the NNC for the period-three XY chain. In this case we choose $N = 120$, the dotted, dotted-dashed and solid lines correspond to $\gamma = 0.1, 0.2, 0.3$, respectively.

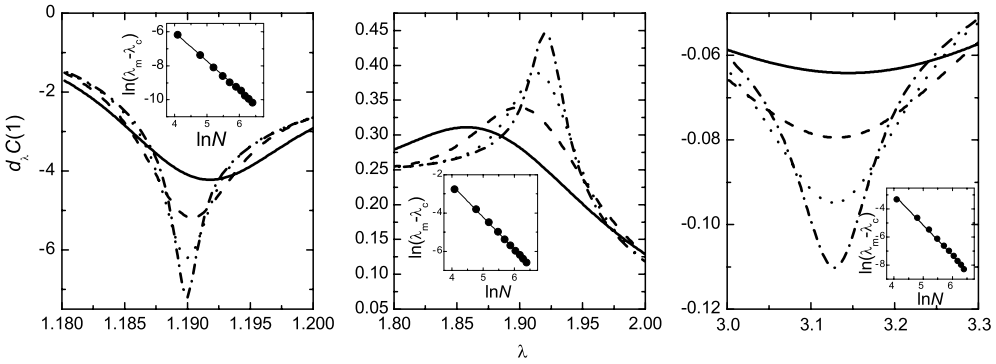

Figure 12. The derivative of the concurrence of the period-three chain at the vicinity of the three critical points. The solid, dashed, dotted and dotted-dashed curves correspond to $N = 60, 120, 240$ and 480, respectively. With the increase in the system size, the position of the minimum or maximum λ_m changes and tends to λ_c as N^α, from first to third critical point $\alpha = -1.71708, -1.67754$ and -2.15696, respectively, where $\gamma = 0.2$.

numerical results for $\beta = 0.5$. For $\beta = 0.5$, the γ_c is equal to 0.246 570 463 568 771. In figure 11, we give the derivative of the concurrence of this case, which clearly shows the critical points.

The period-three case has the similar finite-size scaling law at every critical point as the period-two case, which we can easily see from figures 12 and 13. From figure 13, we can see that the critical exponents at all the three critical points are all the same, $\nu = 1$. So all the critical points belong to the same universality class.

5. Discussion and conclusion

By using the concept of concurrence the entanglement of periodic anisotropic XY chains in a transverse field is studied numerically. We find that the derivative of the NNC in the vicinity of all the critical points for uniform ($T = 1$), period-two ($T = 2$) and period-three ($T = 3$) chains have a similar scaling law, that is, it satisfies the same universality class. For all three cases, the minimum λ_m of the curve at every critical point changes with the increasing system size and tends as

$$\lambda_m - \lambda_c \sim N^\alpha.$$

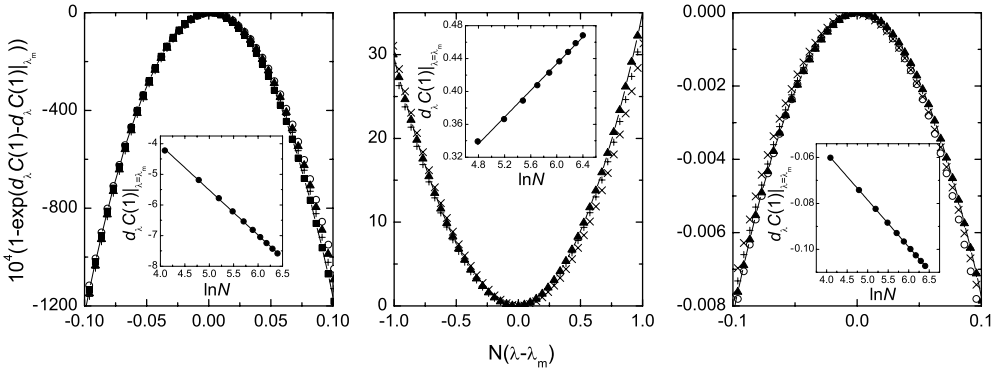

Figure 13. The finite-size scaling is performed for the case of logarithmatic divergence for the period-three chain. At every critical point all the data from $N = 120$ up to $N = 480$ collapse onto a single curve. The inset shows the divergence of the value at the minimum or maximum as the system size increases, $\partial_\lambda C(1)$ changes and tends as $\beta \ln N$, from first to third critical point $\beta = -1.46844$, 0.08108 and -0.02047, respectively, where $\gamma = 0.2$.

Table 1. The index of α at every quantum critical point, $\gamma = 0.2$.

	$\alpha_{\lambda_{C_1}}$	$\alpha_{\lambda_{C_2}}$	$\alpha_{\lambda_{C_3}}$
$T = 1$	$-1.793\,35$	–	–
$T = 2$	$-1.720\,29$	$-1.787\,12$	–
$T = 3$	$-1.717\,08$	$-1.677\,45$	-2.15696

Table 2. The index of κ at every quantum critical point, $\gamma = 0.2$.

	$\kappa_{\lambda_{C_1}}$	$\kappa_{\lambda_{C_2}}$	$\kappa_{\lambda_{C_3}}$
$T = 1$	$-0.305\,04$	–	–
$T = 2$	$-1.245\,09$	$0.020\,48$	–
$T = 3$	$-1.468\,44$	$0.081\,08$	$-0.020\,47$

And the value $\partial_\lambda C(1)$ at the point λ_m logarithmically diverges with increasing system size as

$$\partial_\lambda C(1)|_{\lambda_m} = \kappa \ln N + \text{const.}$$

where α and κ are the functions of γ and β. The typical indexes α and β for $\gamma = 0.2$ and $\beta = 0.5$ are given in tables 1 and 2.

Taking into account the distance of the minimum or maximum of $\partial_\lambda C(1)$ of the three cases from the critical point, it is possible to make all the data for different N collapse approximately onto a single curve in the vicinity of every critical point, respectively. For every critical point, the critical exponent $\nu = 1$, so all the critical points of periodic anisotropic XY chains belong to the same universality class.

Acknowledgments

This work is partly supported by the National Nature Science Foundation of China under Grant Nos 90203009 and 10175035, by the Nature Science Foundation of Jiangsu Province of

China under Grant No. BK2001107, and by the Excellent Young Teacher Program of MOE, People's Republic of China.

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