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Quantum Monte Carlo study on commensurate–incommensurate transition in the spin-1/2 XXZ chain at finite temperatures

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Abstract

A crossover phenomenon of the longitudinal spin–spin correlation function is investigated on the spin-1/2 XXZ chain in a magnetic field at finite temperatures. A commensurate–incommensurate transition of the correlation function in the asymptotic behaviour has been pointed out by Klümper *et al* in the framework of the quantum transfer matrix method. We show the field dependence and the anisotropy-constant dependence of the critical temperature by the quantum transfer matrix method. Using a quantum Monte Carlo method with the continuous time loop algorithm, we directly observe the commensurate–incommensurate transition. Detailed quantum Monte Carlo analyses for the longitudinal spin–spin correlation in both the high and low temperature regions are presented. Especially in the low temperature region, evaluating the precise distance dependence of the correlation function, we prove that the incommensurate oscillation has detectable amplitude, which has not been estimated before. We also estimate the phase factor of the incommensurate oscillation, which accurately coincides with the one from the quantum transfer matrix method.

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1. Introduction

The spin-1/2 XXZ model is one of the most fundamental solvable models describing low-dimensional magnetism, and its physical properties have been studied most extensively [1]. Among them, the evaluation of the correlation function is still a challenging problem. Concerning finite temperature correlations for local operators, the asymptotic behaviour in the vicinity of the critical point (temperature $T = 0$) is systematically determined by a conformal mapping. For a finite magnetic field, the longitudinal spin–spin correlation exponentially decays with an incommensurate oscillation characterized by the Fermi momentum $2k_{\mathrm{F}} < \pi$. Unfortunately, away from the critical point, the above field theoretical approach does not tell the quantitative behaviour of the correlation functions. As an alternative approach, recently the quantum transfer matrix (QTM) method utilizing a lattice path integral formulation has been developed to study finite temperature correlation functions [2–7].

The Hamiltonian of the XXZ model with the nearest-neighbour interaction in a magnetic field is given by

$$\mathcal{H} = J \sum_{j=1}^{L} \left(S_j^x S_{j+1}^x + S_j^y S_{j+1}^y + \Delta S_j^z S_{j+1}^z \right) - h \sum_{j=1}^{L} S_j^z \tag{1}$$

where S_j^x, S_j^y and S_j^z are the spin-1/2 operators acting on the jth site. The periodic boundary condition is adopted in this study. Recently, using the QTM method, Klümper *et al* studied the asymptotic behaviour of the longitudinal spin–spin correlation function

$$C_k = \left\langle S_j^z S_{j+k}^z \right\rangle - \left\langle S_j^z \right\rangle \left\langle S_{j+k}^z \right\rangle \tag{2}$$

for wide ranges of temperature in the antiferromagnetic critical regime: $J > 0$ and $0 < \Delta < 1$ [5]. Here $\langle \cdots \rangle \equiv \mathrm{Tr}(\exp(-\mathcal{H}/k_{\mathrm{B}}T) \cdots)$ denotes the thermal expectation value and a unit $k_{\mathrm{B}} = 1$ is adopted. In general, the asymptotic behaviour of the longitudinal spin–spin correlation function has the form

$$C_{k \gg 1} \sim 2A(T) \cos(2k_{\mathrm{F}}(T)k)\, \mathrm{e}^{-k/\xi(T)}. \tag{3}$$

The temperature dependence of the correlation length $\xi(T)$ and the phase factor $k_{\mathrm{F}}(T)$ of the correlation function (2) in the asymptotic region $k \gg 1$ can be calculated from the ratio of the largest and next leading eigenvalues of the QTM. In the analysis they found the following significant behaviour. At high temperatures, the correlation function simply changes alternately because of the antiferromagnetic interaction. There, the second largest eigenvalue is single and has a negative real value resulting in an exponentially decaying correlation with an alternating oscillation. In this case C_k is given in the form

$$C_{k \gg 1} \sim A(T) \cos(\pi k)\, \mathrm{e}^{-k/\xi(T)} \qquad \text{for} \quad T > T_{\mathrm{c}}. \tag{4}$$

That is, $2k_{\mathrm{F}}(T) = \pi$. Here $A(T)$ is the amplitude of the slowest relaxation and is related to the matrix element of the QTM.

On the other hand, when the temperature decreases, a merging of the second and the third largest eigenvalues occurs at a certain temperature T_{c}. Below T_{c} the two eigenvalues form a complex conjugate pairs resulting in the incommensurate oscillation as expected in the low temperature limit in the field theory. Here $2k_{\mathrm{F}}(T) \neq \pi$.

This transition causes a non-analytic temperature dependence of the correlation length $\xi(T)$ and the phase factor $k_{\mathrm{F}}(T)$. The temperature dependence of $k_{\mathrm{F}}(T)$ obtained by the QTM method is plotted in figure 1. Here we consider the Hamiltonian (1) with the parametrization $J = 2/\sin\gamma$ and $\Delta = \cos\gamma$ as in [5]. We adopt $\gamma = \pi/5$ and $h = 0.1$ as a typical case. The temperature dependence of $\xi(T)$ by the QTM method (open circles) is plotted in figure 2

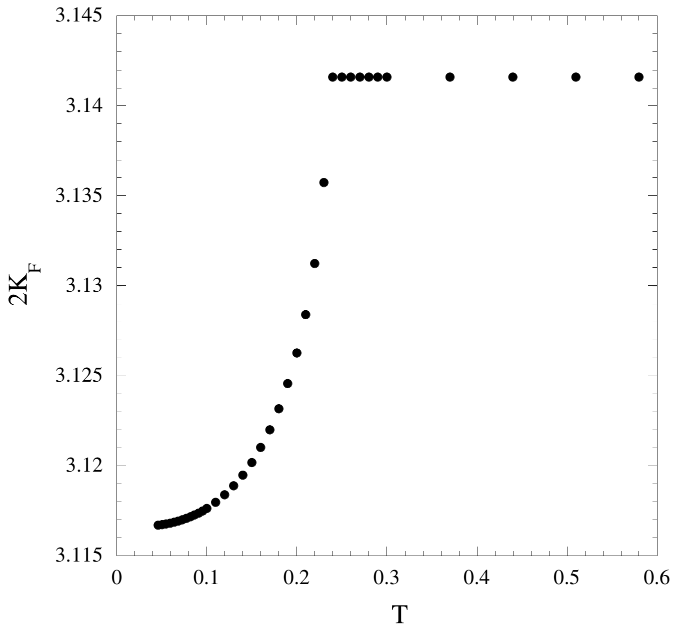

Figure 1. The temperature dependence of the phase factor '$2k_F$' of the correlation function (2) for $J = 2/\sin(\pi/5)$, $\Delta = \cos(\pi/5)$ and $h = 0.1$. The commensurate–incommensurate transition occurs at $T = T_c = 0.233$.

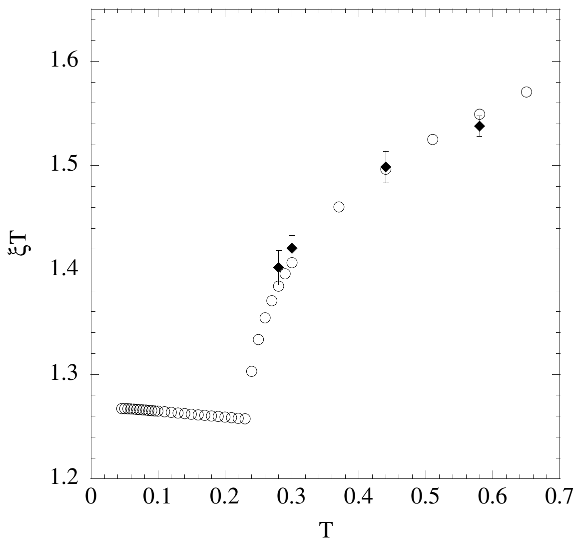

Figure 2. The temperature dependence of the correlation length ξ (multiplied by temperature T) for $J = 2/\sin(\pi/5)$, $\Delta = \cos(\pi/5)$ and $h = 0.1$. The correlation lengths obtained by the QTM method are depicted by the open circles. The crossover temperature T_c is estimated to be $T_c = 0.233$. The results from the QMC method are shown by the closed diamonds.

where the values obtained by the quantum Monte Carlo method (closed diamonds) are also plotted (see the next section). The parameter dependence of the transition temperature is

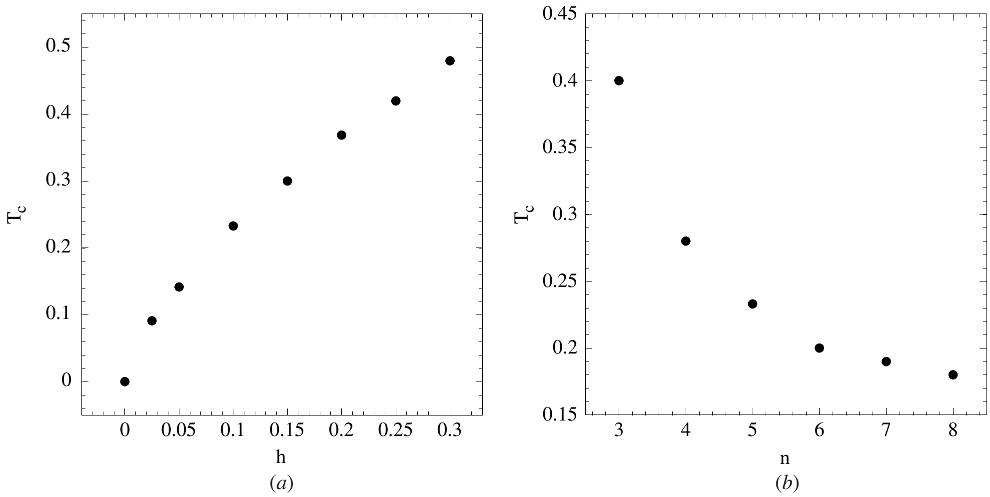

Figure 3. (*a*) The dependence of T_c on h for $J = 2/\sin(\pi/5)$ and $\Delta = \cos(\pi/5)$. (*b*) The dependence of T_c on Δ for $J = 2/\sin(\pi/5)$ and $h = 0.1$. The label n on the horizontal axis is defined as $\Delta = \cos(\pi/n)$.

an interesting problem. The field (h) dependence of T_c by the QTM method is shown in figure 3(*a*) and the anisotropy-constant (Δ) dependence of T_c by the QTM method is also shown in figure 3(*b*) where n is defined as $\Delta = \cos(\pi/n)$. Here we find that the transition temperature increases when the field (h) increases, while the transition temperature decreases when the anisotropy constant (Δ) increases.

This transition indicates that a commensurate–incommensurate transition driven by temperatures takes place in the XXZ model with an external field. Note that this crossover phenomenon does not occur without magnetic fields, where the asymptotic form of the correlation function always takes the form (4).

The QTM method clearly revealed that the commensurate–incommensurate transition due to temperature occurs in the analysis of the correlation length and the phase factor. The amplitude of the relevant behaviour is given by $A(T)$. However, it is difficult to estimate this amplitude in the QTM method explicitly. It is interesting to study how this new type of phenomenon in the quantum spin system appears in observations. If the amplitude $A(T)$ has a very small value, we cannot observe the incommensurate oscillation practically. Indeed, estimation of $A(T)$ has not been done yet.

To investigate whether the amplitude $A(T)$ is large enough to detect the incommensurate oscillation is a very significant problem not only in the theoretical sense but also in the experimental sense. Furthermore, it is interesting to figure out how we can observe the oscillation decay in an explicit way.

In order to study this problem, we exploit the quantum Monte Carlo (QMC) method with the continuous time loop algorithm [8–12] and directly evaluate the distance dependence of the correlation function at both high and sufficiently low temperatures.

The loop algorithm, which is a kind of cluster algorithm, has the following advantages over the conventional one based on local updates of spin configurations (referred to as the world line algorithm [13]). First, serious long autocorrelation problems peculiar to the conventional algorithm especially at low temperatures are overcome in the loop algorithm updating spin configurations by changes of non-local 'loop'. This method allows us to simulate the system in the very low temperature region efficiently. Second, we can avoid numerical errors involved in the extrapolation of the Trotter limit, introducing the continuous time method [12] into the loop algorithm. We can directly simulate the Trotter limit. Recently, these advantages of this method have been shown in many contexts in spin systems [11].

This QMC method enables us to evaluate the correlation function at low temperatures, and we obtain an explicit example of the commensurate–incommensurate transition of the correlation function. We show that the incommensurate oscillation is detectable by estimating the amplitude $A(T)$ explicitly which has not been estimated before. We also estimate the phase factor $k_{\mathrm{F}}(T)$, which agrees with the estimation by the QTM method.

2. Monte Carlo simulation

In order to estimate the correlation length and the phase factor, we obtain the correlation function C_k. Because of the finite value of h the magnetization $m = \langle S_j^z \rangle$ itself is not zero. In order to avoid the finite-size effect and to separate the constant part $\langle S_j^z \rangle \langle S_{j+k}^z \rangle$ from the asymptotic form of $\langle S_j^z S_k^z \rangle$ precisely, we investigate in a long chain with as much precision as possible.

We use a periodic chain with $L = 180$ sites for the high temperature region ($T > T_{\mathrm{c}}$). This chain length is sufficiently long compared with the correlation length ($\xi < 6$) evaluated by the QTM method ($T > T_{\mathrm{c}}$).

To obtain good statistics, we adopt the following procedure. We performed 100 000 Monte Carlo steps (MCS) to reach equilibrium. Here the MCS means the number of updates of whole spins in the 2D configuration space (lattice space and imaginary time space). Then, we performed 100 000 MCS for one sampling for the evaluation of C_k. We obtain the correlation function C_k by averaging over ten independent samplings.

In general, the efficiency of the Monte Carlo method with the loop algorithm becomes worse when the magnetic field becomes strong [14]. However, in the present case, the value $h/J \simeq 0.0294$ is very small and we do not suffer from this difficulty in practice. Indeed, we checked convergence for the lowest temperature case by performing a long run with more than 1000 000 MCS.

We estimate the correlation length ξ in the following procedure. First, we plot $\ln((-1)^k C_k) = \ln |C_k|$ as a function of k. Then, we estimate the slope of $\ln |C_k|$ by the least-squares fitting for the following two sets of sites: $k = i, i+2, i+4, i+6$ and $k = i+1, i+3, i+5, i+7$, where i is a certain site. Averaging the slopes in these two cases, we obtain i-dependent 'correlation length' ξ_i. We take a saturated value of ξ_i for large i as the correlation length ξ, although the correlation becomes small and the statistics of data becomes worse when i increases. We show the i-dependence of $\xi_i T$ at $T = 0.44$ in figure 4 as a typical example. We take the average value of $\xi_i T$ over six independent trials, where one trial means an estimation of ξ_i for $\{C_k\}$ obtained by averaging over ten independent samplings. Because the procedure to obtain $\xi_i T$ contains nonlinear operations, it is complicated to define the error bar. Here, we simply define the error bar as the standard deviations of distribution of the data. In this case, the saturated value is $\xi T = 1.50$ which agrees well with the result from the QTM method. The value is plotted in figure 2 by a closed diamond.

In figure 5, we plot $\ln |C_k|$ as a function of k. With the value of ξ obtained by the above procedure, the data points are well superimposed for large k (>10). Similarly, the correlation lengths ξ are estimated at $T = 0.28$, 0.30 and 0.58, and are depicted by closed diamonds in figure 2. Here we have confirmed that our method works in practice to obtain the correlation length in the temperature region $T \geqslant 0.28$.

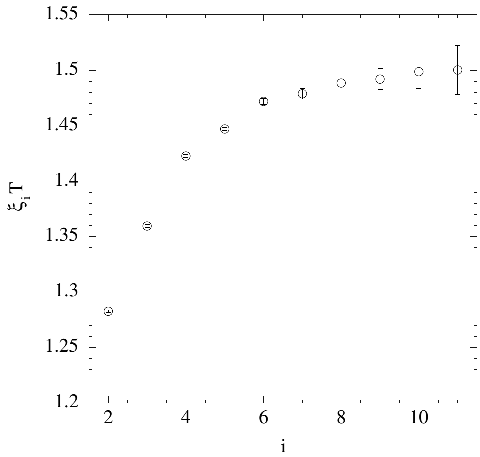

Figure 4. The *i*-dependence of the correlation length (multiplied by temperature T) for the system size $L = 180$ and $T = 0.44$. The saturated value is estimated to be $\xi T = 1.50$.

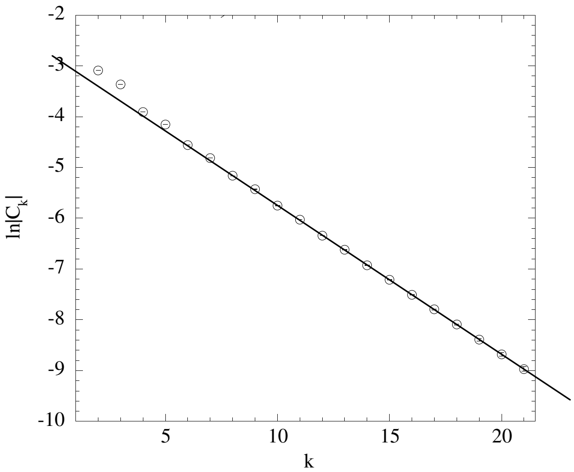

Figure 5. $\ln |C_k|$ as a function of k for the system $L = 180$ at $T = 0.44$.

However, we find that C_k does not show a simple exponential relaxation when the temperature comes closer to the critical point. In figure 6, we depict a typical example at $T = 0.26$. We have investigated the correlation function very carefully and confirmed that the non-single exponential relaxation is not due to insufficient data sampling. At the critical temperature, the second and third eigenvalues are degenerate. Thus, near the critical point, there are two relaxation modes which have nearly the same correlation length. This fact may cause the strange behaviour of C_k. At the present stage we do not manage to estimate ξ from the data. We cannot obtain the critical behaviour of ξ, which is left for future study.

Next, we study the correlation function at low temperatures ($T < T_c$), where we expect the incommensuration of the correlation function. Near the critical point, the period of the oscillation is very long and the correlation length is relatively small in the analysis of the QTM method. Thus, it is difficult to observe the change due to the phase factor, $\cos(2k_F(T)k)$, and determine ξ and k_F by the QMC method. In order to find the incommensuration, we

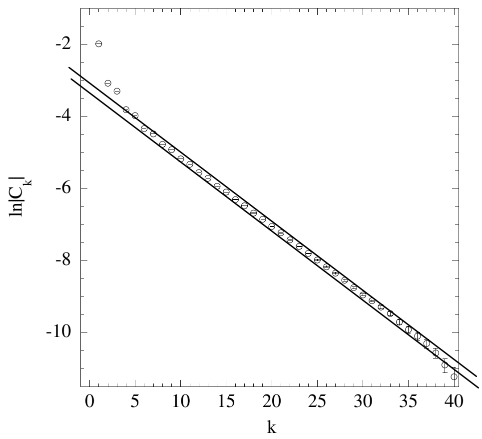

Figure 6. $\ln|C_k|$ as a function of k for the system $L = 180$ at $T = 0.26$. Two parallel linear lines with the inclination $-1/\xi$ evaluated by the QTM method are also shown.

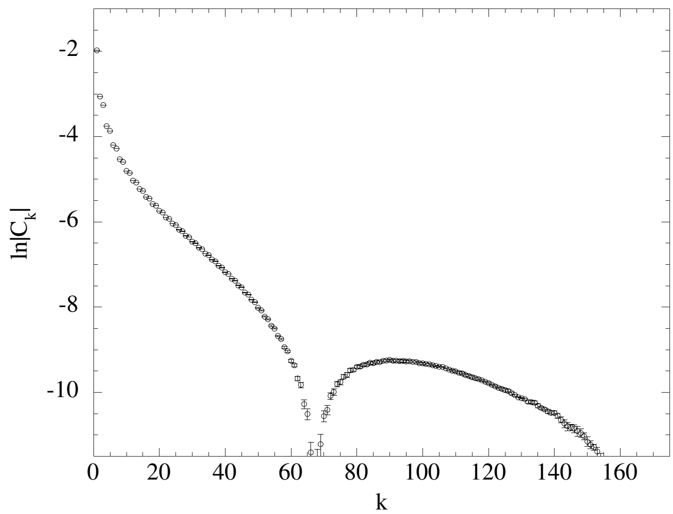

Figure 7. $\ln|C_k|$ as a function of k for the system $L = 504$ at $T = 0.046$. The divergence is observed around $k = 65$.

study the correlation function at a rather low temperature, although it takes longer CPU time at lower temperatures. Concretely, we exploit $T = 0.046$. Here we adopt a periodic chain with $L = 504$ sites, which is sufficiently long compared with the correlation length $\xi \simeq 27.55$ evaluated by the QTM method (see figure 2). We estimate the correlation function C_k averaging over four independent samplings each of which consists of 100 000 MCS.

In figure 7 we plot $\ln|C_k|$. We find that $\ln|C_k|$ diverges around the 65th site. From equation (3), it is natural to consider that this divergence occurs at the position of the node of $\cos(2k_{\rm F}(T)k)$. Therefore, this divergence of $\ln|C_k|$ indicates the incommensurate oscillation of the correlation function. Using this position (65th site), we evaluate the phase factor $2k_{\rm F}$ as

$$2k_{\rm F} = \pi - \pi/(2 \times 65) = 3.1174. \tag{5}$$

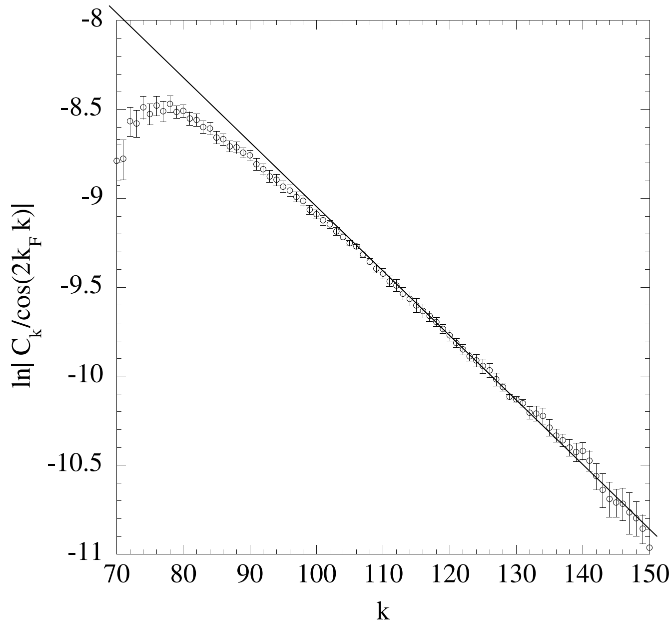

Figure 8. $\ln(|C_k/\cos(2k_F k)|)$ as a function of k for the system with $L = 504$ at $T = 0.046$. The linear line with the inclination $-1/\xi$ evaluated by the QTM method is also shown.

This value agrees well with the QTM result $2k_F = 3.1167$, from which the position of node is evaluated to be around the 63rd site. Although the value of the correlation function is rather small $\sim e^{-10}$, this is the first explicit observation of the incommensutate behaviour of the correlation function.

Next, we evaluate the correlation length ξ at this temperature. We plot $\ln(|C_k/\cos(2k_F k)|)$ as a function of k in figure 8. The result shows that the correlation function decays in a single exponential form for large distance, and its exponent agrees with the reciprocal correlation length $-1/\xi$ calculated by the QTM method which is shown by the linear line in figure 8. Thus, we also confirmed the result of the QTM in the low temperature region.

3. Summary

The commensurate–incommensurate transition which was predicted by the QTM method has been investigated. We have shown the field dependence and anisotropy-constant dependence of the transition temperature in the QTM method: the transition temperature (T_c) increases when the field (h) increases or the anisotropy constant (Δ) decreases.

Using the QMC method with the continuous time loop algorithm, we have studied the longitudinal spin–spin correlation function of the XXZ model in an external field at finite temperatures.

The correlation functions with commensurate and incommensurate oscillations have been explicitly observed in the QMC method at high and low temperatures, respectively. Although estimation of the absolute value of the correlation function (amplitude) is difficult in the QTM method and has not been investigated before, the present finding proves that the incommensurate oscillation is detectable in practical observation. We have also estimated the correlation length and the phase factor of the correlation function, which agree with the results evaluated by the QTM method. Thus, we found the commensurate and incommensurate regions at temperatures apart from the critical point. However, it was found very difficult to determine ξT and k_{F} in the vicinity of T_{c}, although we investigated the correlation function carefully. There the correlation function shows non-single exponential relaxation. This feature may be related to a critical property of the present transition, but it is left for a challenging problem in the future.

Finally, let us remark that similar crossover phenomena due to the temperature and the external field have also been found in the t–J chain [15] recently. More generally commensurate–incommensurate transitions at finite temperatures have been reported in other spin chains with competing interactions [16, 17]. It would be an interesting problem to find a common feature among these transitions.

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