

Pair correlations for double-chain and triple-chain Ising models with competing interactions

Terufumi Yokota

Japan Atomic Energy Research Institute, Tokai, Ibaraki 319-11, Japan
 (Received 13 September 1988; revised manuscript received 18 January 1989)

Pair correlations for the Ising model on a triple-chain with a crossed second-neighbor interaction are obtained analytically and their asymptotic decay for the large spin separation is investigated. The change in the nature of the long-distance asymptotic decay is observed in small regions of the parameter space, where the interactions are competing. This change is caused by the interchange of the second largest eigenvalue of the transfer matrix in absolute value. The results are compared with the double-chain case to study the effect of the frustration in the triangle made of three nearest-neighbor spins on different chains when the interchain nearest-neighbor interaction is antiferromagnetic.

Spin systems with competing interactions have been studied for a long time. Some two-dimensional Ising models with both ferromagnetic and antiferromagnetic interactions have been solved exactly. Reentrant phenomena are observed on the lattice studied in Refs. 1 and 2. Changes in the nature of the short-range order occur both on this lattice and on the anisotropic triangular lattice, although the manners of the changes are different.³ Such phenomena are also observed for the corresponding one-dimensional models.⁴ As to the two-dimensional Ising model with crossed second-neighbor competing interactions, the exact solution has not yet been obtained but reentrant phenomena are observed in the double-chain approximation.⁵ The corresponding one-dimensional model has been investigated focusing on the effect of competing interactions.⁶ Furthermore, the antiferromagnetic Ising model on the triangular lattice⁷ is the subject of renewed interest⁸ from a viewpoint of the frustration.⁹

Here we calculate pair correlations of a triple-chain Ising model with a crossed second-neighbor interaction in zero field, analytically. In the case of the one-dimensional

models without crossed second-neighbor interactions, there is a temperature at which the nature of the short-range order changes abruptly.⁴ So it would be interesting to see the effect of the crossed interaction on the nature of the short-range order. In contrast with the case without crossed second-neighbor interactions, clear changes in the short-range order are not observed. However, the change in the nature of the long-distance asymptotic decay for the pair correlation is preserved when interactions are competing. The results are compared with the double-chain case to study the effect of the frustration which lives in the triangle made of three nearest-neighbor spins on different chains when the interchain nearest-neighbor interaction is antiferromagnetic.

In Fig. 1, we show the double chain and the triple chain studied here. The chains are infinite and the periodic boundary condition is assumed. In the triple chain, the third chain is also a nearest neighbor of the first chain so that the periodic boundary condition is assumed also in the direction perpendicular to the chains. The Hamiltonians for the double chain and the triple chain are given by

$$H^{(2)} = \sum_{i=1}^N (-J_1 S_{i,1} S_{i+1,1} - J_1 S_{i,2} S_{i+1,2} - J_2 S_{i,1} S_{i,2} - J_3 S_{i,1} S_{i+1,2} - J_3 S_{i,2} S_{i+1,1}), \tag{1}$$

and

$$H^{(3)} = - \sum_{i=1}^N [J_1 (S_{i,1} S_{i+1,1} + S_{i,2} S_{i+1,2} + S_{i,3} S_{i+1,3}) + J_2 (S_{i,1} S_{i,2} + S_{i,2} S_{i,3} + S_{i,3} S_{i,1}) + J_3 (S_{i,1} S_{i+1,2} + S_{i+1,1} S_{i,2} + S_{i,2} S_{i+1,3} + S_{i+1,2} S_{i,3} + S_{i,3} S_{i+1,1} + S_{i+1,3} S_{i,1})]. \tag{2}$$

The pair correlations for the triple-chain Ising model are obtained by the transfer-matrix method as in the double-chain case.⁶ The transfer-matrix T is given by

$$T = \begin{pmatrix} \uparrow\uparrow\uparrow & \uparrow\uparrow\downarrow & \uparrow\downarrow\downarrow & \downarrow\downarrow\downarrow & \uparrow\downarrow\downarrow & \uparrow\downarrow\downarrow & \downarrow\downarrow\downarrow & \downarrow\downarrow\downarrow & \downarrow\downarrow\downarrow \\ \left(\begin{array}{cccccccc} a & b & b & b & c & c & c & d \\ b & e & f & f & g & g & h & c \\ b & f & e & f & g & h & g & c \\ b & f & f & e & h & g & g & c \\ c & g & g & h & e & f & f & b \\ c & g & h & g & f & e & f & b \\ c & h & g & g & f & f & e & b \\ d & c & c & c & b & b & b & a \end{array} \right) \begin{array}{l} \uparrow\uparrow\uparrow \\ \uparrow\uparrow\downarrow \\ \uparrow\downarrow\downarrow \\ \downarrow\downarrow\downarrow \\ \uparrow\downarrow\downarrow \\ \uparrow\downarrow\downarrow \\ \downarrow\downarrow\downarrow \\ \downarrow\downarrow\downarrow \end{array}, \tag{3}$$

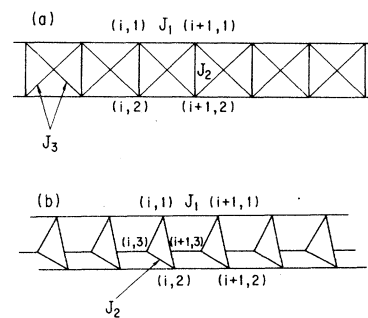


FIG. 1. Symmetric double chains and symmetric triple chains in which the third chain is also a nearest neighbor of the first chain. Although there are crossed second-neighbor interactions, they are omitted in (b) for simplicity.

where $a = \exp(3v_1 + 3v_2 + 6v_3)$, $b = \exp(v_1 + v_2 + 2v_3)$, $c = \exp(-v_1 + v_2 - 2v_3)$, $d = \exp(-3v_1 + 3v_2 - 6v_3)$, $e = \exp(3v_1 - v_2 - 2v_3)$, $f = \exp(-v_1 - v_2 + 2v_3)$, $g = \exp(v_1 - v_2 - 2v_3)$, and $h = \exp(-3v_1 - v_2 + 2v_3)$ with the notation of $v_i \equiv \beta J_i$. Taking account of the geometrical symmetry under the mutual permutation of the three chains and the internal spin symmetry, we can diagonalize the 8×8 transfer matrix by a unitary transformation $U^+ T U$ with

$$U = \frac{1}{\sqrt{6}} \begin{pmatrix} \sqrt{3} \sin \theta_1 & \sqrt{3} \cos \theta_1 & 0 & 0 & \sqrt{3} \cos \theta_2 & 0 & 0 & -\sqrt{3} \sin \theta_2 \\ \cos \theta_1 & -\sin \theta_1 & 1 & 1 & \sin \theta_2 & \omega^2 & \omega & \cos \theta_2 \\ \cos \theta_1 & -\sin \theta_1 & \omega & \omega^2 & \sin \theta_2 & \omega & \omega^2 & \cos \theta_2 \\ \cos \theta_1 & -\sin \theta_1 & \omega^2 & \omega & \sin \theta_2 & 1 & 1 & \cos \theta_2 \\ \cos \theta_1 & -\sin \theta_1 & \omega^2 & \omega & -\sin \theta_2 & -1 & -1 & -\cos \theta_2 \\ \cos \theta_1 & -\sin \theta_1 & \omega & \omega^2 & -\sin \theta_2 & -\omega & -\omega^2 & -\cos \theta_2 \\ \cos \theta_1 & -\sin \theta_1 & 1 & 1 & -\sin \theta_2 & -\omega^2 & -\omega & -\cos \theta_2 \\ \sqrt{3} \sin \theta_1 & \sqrt{3} \cos \theta_1 & 0 & 0 & -\sqrt{3} \cos \theta_2 & 0 & 0 & \sqrt{3} \sin \theta_2 \end{pmatrix}, \quad (4)$$

where $\omega = \exp(2\pi i/3)$ is a cubic root of 1, and

$$\begin{aligned} \sin \theta_1 &= [(\sqrt{D_1} + a + d - e - 2f - 2g - h)/2\sqrt{D_1}]^{1/2}, \\ \cos \theta_1 &= \sqrt{6}(b+c)[(\sqrt{D_1} + a + d - e - 2f - 2g - h)\sqrt{D_1}]^{-1/2}, \\ \sin \theta_2 &= [(\sqrt{D_2} - a + d + e + 2f - 2g - h)/2\sqrt{D_2}]^{1/2}, \\ \cos \theta_2 &= \sqrt{6}(b-c)[(\sqrt{D_2} - a + d + e + 2f - 2g - h)\sqrt{D_2}]^{1/2}, \end{aligned} \quad (5)$$

with

$$D_1 = (a + d - e - 2f - 2g - h)^2 + 12(b + c)^2$$

and

$$D_2 = (-a + d + e + 2f - 2g - h)^2 + 12(b - c)^2.$$

In order to obtain the pair correlations, we introduce the following layer spin matrix σ_a as in the double-chain case:⁶

$$\sigma_1 = \begin{pmatrix} 1 & & & & & & & \\ & 1 & & & & & & \\ & & 1 & & & & & \\ & & & -1 & & & & \\ & & & & 1 & & & \\ & & & & & -1 & & \\ & & & & & & 1 & \\ & & & & & & & -1 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 1 & & & & & & & \\ & 1 & & & & & & \\ & & -1 & & & & & \\ & & & 1 & & & & \\ & & & & -1 & & & \\ & & & & & 1 & & \\ & & & & & & -1 & \\ & & & & & & & 1 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & & & & & & & \\ & -1 & & & & & & \\ & & 1 & & & & & \\ & & & -1 & & & & \\ & & & & 1 & & & \\ & & & & & -1 & & \\ & & & & & & 1 & \\ & & & & & & & -1 \end{pmatrix}. \quad (6)$$

The pair correlations for $j < k$ are given by

$$\langle S_{j,\alpha} S_{k,\beta} \rangle = \lim_{N \rightarrow \infty} \frac{\text{Tr}(T^{j-1} \sigma'_\alpha T^{k-j} \sigma'_\beta T^{N-k+1})}{\text{Tr}(T^N)} = \lim_{N \rightarrow \infty} \frac{\text{Tr}(\Lambda^{j-1} \sigma'_\alpha \Lambda^{k-j} \sigma'_\beta \Lambda^{N-k+1})}{\lambda_{1,+}^N}, \quad (7)$$

where $\sigma'_\alpha = U^+ \sigma_\alpha U$ and

$$\Lambda = U^+ T U = \begin{pmatrix} \lambda_{1,+} & & & & & & & \\ & \lambda_{1,-} & & & & & & \\ & & \lambda_{3,+} & & & & & \\ & & & \lambda_{3,+} & & & & \\ & & & & \lambda_{2,+} & & & \\ & & & & & \lambda_{3,-} & & \\ & & & & & & \lambda_{3,-} & \\ & & & & & & & \lambda_{2,-} \end{pmatrix}, \quad (8)$$

with the following eigenvalues of the transfer matrix:

$$\lambda_{1,\pm} = (a+d+e+2f+2g+h \pm \sqrt{D_1})/2, \quad \lambda_{2,\pm} = (a-d+e+2f-2g+h \pm \sqrt{D_2})/2, \quad \lambda_{3,\pm} = e-f \pm (h-g). \quad (9)$$

The final result for the pair correlations is given by

$$\langle S_{j,1} S_{k,1} \rangle = (\sin\theta_1 \cos\theta_2 + \frac{1}{3} \cos\theta_1 \sin\theta_2)^2 \left(\frac{\lambda_{2,+}}{\lambda_{1,+}} \right)^{k-j} + (-\sin\theta_1 \sin\theta_2 + \frac{1}{3} \cos\theta_1 \cos\theta_2)^2 \left(\frac{\lambda_{2,-}}{\lambda_{1,+}} \right)^{k-j} + \frac{8}{9} \cos^2\theta_1 \left(\frac{\lambda_{3,-}}{\lambda_{1,+}} \right)^{k-j}, \quad (10)$$

$$\langle S_{j,1} S_{k,2} \rangle = (\sin\theta_1 \cos\theta_2 + \frac{1}{3} \cos\theta_1 \sin\theta_2)^2 \left(\frac{\lambda_{2,+}}{\lambda_{1,+}} \right)^{k-j} + (-\sin\theta_1 \sin\theta_2 + \frac{1}{3} \cos\theta_1 \cos\theta_2)^2 \left(\frac{\lambda_{2,-}}{\lambda_{1,+}} \right)^{k-j} - \frac{4}{9} \cos^2\theta_1 \left(\frac{\lambda_{3,-}}{\lambda_{1,+}} \right)^{k-j}.$$

The ground states of the two systems can be obtained easily from the energy consideration. The ground-state phase diagrams for $J_1 > 0$ are shown in Fig. 2(a) for the double chain and in Fig. 2(b) for the triple chain. The notation of $J'_i = J_i/J_1$ is used. We will discuss the case of $J_1 > 0$ in the following because results for $J_1 < 0$ are sim-

ply obtained from the symmetry under $J_1 \leftrightarrow -J_1$, $J_2 \leftrightarrow J_2$, and $J_3 \leftrightarrow -J_3$. The configuration attached by the transfer-matrix element f in (b) is one of the infinite number of possible configurations.

When the interactions are competing, there may be a temperature T^* at which the nature in the long-distance asymptotic decay of the pair correlation changes. This phenomenon has been observed in similar one-dimensional systems without crossed second-neighbor interactions.⁵ Although such a change may not have significance when the correlation length is not large, there exist small regions of parameters near the ground-state transition lines where the change in the long-distance asymptotic decay occurs at a sufficiently low temperature and the correlation length is large. In this model, the change is induced by the interchange of the second largest eigenvalue of the

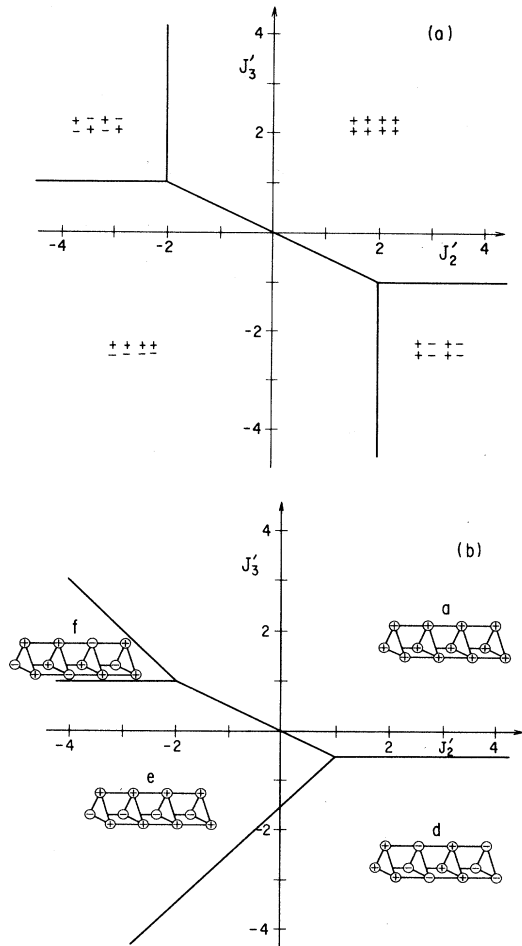


FIG. 2. Ground-state phase diagrams for (a) the double-chain Ising model and (b) the triple-chain Ising model in zero field. $J_1 > 0$ and the notations of $J'_i = J_i/J_1$ are used. The phases for the triple chain are denoted by the transfer-matrix elements. The configuration attached by the transfer-matrix element f is one of the infinite possible configurations.

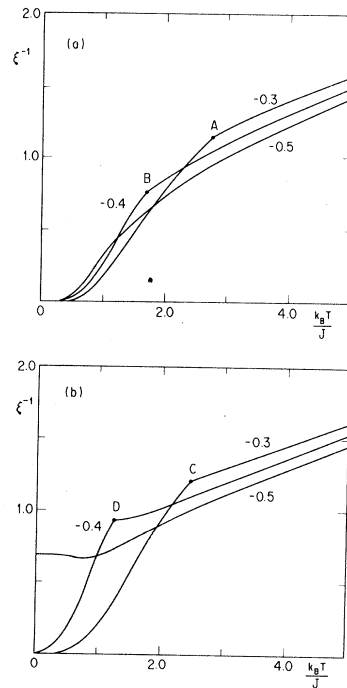


FIG. 3. Correlation length ξ as a function of T for $J_1 = J_2 = J$ and $J_3 = -0.3, -0.4, \text{ and } -0.5$. The double-chain and the triple-chain cases are shown in (a) and (b), respectively. T^* at $A, B, C, \text{ and } D$ are given by 2.7829, 1.6813, 2.4842, and 1.2591, respectively.

transfer matrix in absolute value. The asymptotic decay of the correlation function for the large spin separation r is approximated by $e^{-r/\xi}$. The correlation length ξ may be defined by $\xi^{-1} = \ln(\min |\lambda_{\max}/\lambda_i|)$, where λ_i is the eigenvalue of the transfer matrix except the largest eigenvalue λ_{\max} . In Fig. 3, we show ξ^{-1} as a function of T for $J'_2 = 1$ and $J'_3 = -0.3, -0.4,$ and -0.5 .

In the triple chain, the triangle made of three spins $S_{i,1}$, $S_{i,2}$, and $S_{i,3}$ is frustrated for $J'_2 < 0$. On the other hand, such an effect is absent in the double chain. So it would be interesting to compare the two cases. To obtain the long-distance asymptotic decay of the pair correlation for the double chain, we reproduce pair correlations for the double chain which have been obtained by Kalok and de Menezes⁶ and have the following forms:

$$\langle S_{j,1} S_{k,1} \rangle = \sin^2 \xi \left(\frac{\lambda_4^{(2)}}{\lambda_1^{(2)}} \right)^{k-j} + \cos^2 \xi \left(\frac{\lambda_3^{(2)}}{\lambda_1^{(2)}} \right)^{k-j}, \quad (11)$$

$$\langle S_{j,1} S_{k,2} \rangle = \sin^2 \xi \left(\frac{\lambda_4^{(2)}}{\lambda_1^{(2)}} \right)^{k-j} - \cos^2 \xi \left(\frac{\lambda_3^{(2)}}{\lambda_1^{(2)}} \right)^{k-j},$$

where

$$\sin \xi = \frac{1}{\sqrt{2}} \frac{\sqrt{D} + a + c - d - e^{1/2}}{\sqrt{D}}, \quad (12)$$

$$\cos \xi = 2\sqrt{2} [(\sqrt{D} + a + c - d - e)\sqrt{D}]^{-1/2},$$

and

$$\begin{aligned} \lambda_1^{(2)} &= \frac{a + c + d + e + \sqrt{D}}{2}, \\ \lambda_3^{(2)} &= d - e, \\ \lambda_4^{(2)} &= a - c, \end{aligned} \quad (13)$$

with $a = \exp(2v_1 + v_2 + 2v_3)$, $c = \exp(-2v_1 + v_2 - v_3)$, $d = \exp(2v_1 - v_2 - 2v_3)$, $e = \exp(-2v_1 - v_2 + 2v_3)$, and $D = (a + c - d - e)^2 + 16$. The change in the long-distance asymptotic decay of the pair correlation for the triple chain can be obtained by using (10).

In Fig. 4, we hatch parameter regions where such a change in the long-distance asymptotic decay happens together with the schematic description of the change in the dominant part of the short-range order although the description by the short-range order is only by convenience because the changes in the short-range order cannot be seen clearly. In this figure, the interchange of the eigenvalue of the second largest absolute value is also shown. This eigenvalue controls the long-distance asymptotic decay of the pair correlation. Because of the frustrated triangle mentioned above, the triple-chain case is rather different from the double-chain case especially for $J'_2 < 0$. In the double-hatched region, we observe successive changes in the nature of the long-distance asymptotic

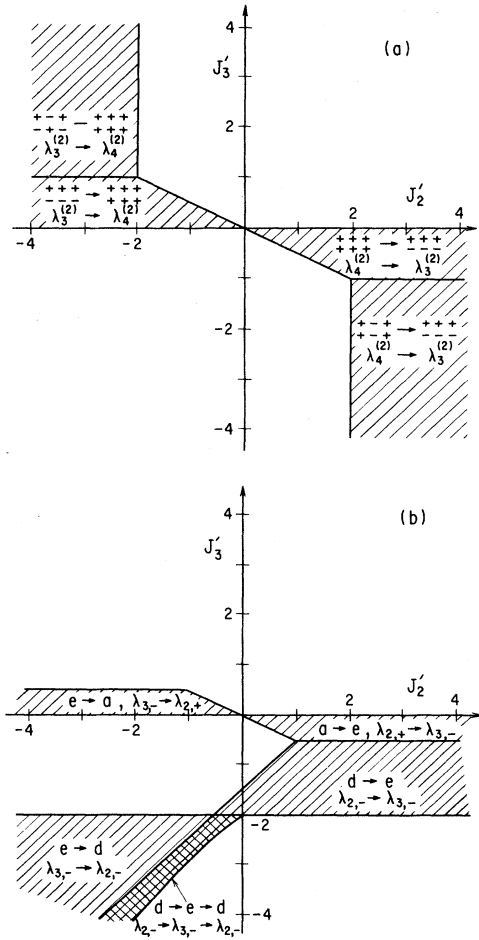


FIG. 4. In hatched regions, there is a temperature at which the nature in the long-distance asymptotic decay of the pair correlation changes as indicated schematically by using the dominant part of the short-range order. The changes are also described by the interchange of the eigenvalue of the second largest absolute value. In (b), the same abbreviated notations by using the transfer-matrix elements as in Fig. 2(b) are employed. The double-chain and the triple-chain cases are shown in (a) and (b), respectively. In the double-hatched region of (b), successive changes in the nature of the asymptotic decay are observed.

decay.

In conclusion, we have obtained pair correlations of a triple-chain Ising model with a crossed second-neighbor interaction, analytically. Effects of competing interactions and the frustrated triangle on the change in the long-distance asymptotic decay of the pair correlation have been investigated.

¹V. G. Vaks, A. I. Larkin, and N. Ovchinnikov, Zh. Eksp. Teor. Fiz. **49**, 1180 (1965) [Sov. Phys. JETP **22**, 820 (1966)].

²T. Chikyu and M. Suzuki, Prog. Theor. Phys. **78**, 1242 (1987).

³J. Stephenson, Phys. Rev. B **1**, 4405 (1970).

⁴J. Stephenson, Can. J. Phys. **48**, 1724 (1970).

⁵T. Yokota, Phys. Rev. B **39**, 523 (1989).

⁶K. Kalok and L. C. de Menezes, Z. Phys. B **20**, 223 (1975).

⁷G. M. Wannier, Phys. Rev. **79**, 357 (1950).

⁸Recent intensive studies on the subject are initiated by the mean-field work of M. Mekata, J. Phys. Soc. Jpn. **42**, 76 (1977).

⁹See, e.g., R. Liebmann, *Statistical Mechanics of Periodic Frustrated Ising Systems* (Springer-Verlag, Berlin, 1986).