

AUTOCORRELATION FUNCTION OF THE
HEISENBERG FERROMAGNET AT ELEVATED TEMPERATURE

T. MORITA^{*}, K. KOBAYASHI[†], Y. ABE[‡], and S. KATSURA[†]

^{}Department of Applied Science, [†]Department of Applied Physics*

[‡]Department of Physics, Tohoku University, Sendai, Japan

The coefficients of the short time expansion of the autocorrelation function of the anisotropic Heisenberg model are given up to the sixth order for the square, simple cubic and body-centered cubic lattices, and up to the tenth order for the linear chain.

Since Van Hove [1] gave the relation between space-time correlation functions of spins and the differential scattering cross section of the neutron diffraction, many investigations were carried out on the correlation functions of spins. We consider this function for the anisotropic Heisenberg model with nearest neighbor interaction of $S=1/2$. The Hamiltonian of this system is given by

$$H = \sum_i \sum_{\Delta} (J_{\perp} s_i^+ s_{i+\Delta}^- + J_{\parallel} s_i^z s_{i+\Delta}^z). \quad (1)$$

de Gennes [2] obtained the second and the fourth moment of $\langle S_k^z S_{-k}^z \rangle_{\omega}$ at infinite high temperature for the polycrystal, and Marshall [3] the same quantities for the isotropic single crystal. McFadden and Tahir-Kehli [4,5] calculated the sixth moment for the isotropic case and the second and the fourth for the anisotropic model. Spin correlation functions for one-dimensional XY model was exactly obtained by Katsura, Horiguchi and Suzuki [6]. Nakamura [7] calculated the moments of the autocorrelation function up to the eighth order for the one-dimensional isotropic case.

The zz -spin correlation function is expanded in powers of time t as follows;

$$\begin{aligned} \langle s_{\ell}^z(0) s_0^z(t) \rangle &= \frac{1}{4} - \frac{t^2}{2!} \langle s_{\ell}^z [H, [H, s_0^z]] \rangle \\ &+ \frac{t^4}{4!} \langle s_{\ell}^z [H, [H, [H, [H, s_0^z]]]] \rangle + \dots \quad (2) \end{aligned}$$

The non-vanishing terms in H in the commutator $[H, s_0^z]$ are $s_0^+ s_{0+\Delta}^-$ and $s_{0-\Delta}^+ s_0^-$. Drawing graphs which correspond to non-vanishing terms after taking the commutator $[H, \quad]$ in the memory of the computer, we can obtain the coefficients of t^{2n} in the correlation function $\langle s_{\ell}^z(0) s_0^z(t) \rangle$.

In this paper we list the short time expansion of the autocorrelation function of the anisotropic Heisenberg model at infinite temperature up to the sixth order for the linear, square, simple cubic, and body-centered cubic lattices, and the coefficients of the eighth and tenth orders for the linear

lattice. The results are given by

$$\begin{aligned}
\langle s_0^z(0) s_0^z(t) \rangle &= \frac{1}{4} - \frac{t^2}{2!} \frac{z}{2} J_{\perp}^2 \\
&+ \frac{t^4}{4!} \left[\left(2z + \frac{5}{2} z_2 \right) J_{\perp}^4 + z_2 J_{\perp}^2 J_{\parallel}^2 \right] \\
&- \frac{t^6}{6!} \left[(8z + 33z_2 + 9z_3 + 28v_{3,1}) J_{\perp}^6 + \left(\frac{27}{2} z_2 + 14z_3 + 11v_{3,1} - 7v_4 \right) J_{\perp}^4 J_{\parallel}^2 \right. \\
&\left. + (z_2 + 3z_3 + 6v_{3,1}) J_{\perp}^2 J_{\parallel}^4 \right] + O(t^8), \quad (3)
\end{aligned}$$

where z and v_4 are the number of nearest neighbor lattice sites and squares, respectively; $z=2, 4, 6, 8$ and $v_4=0, 4, 12, 48$ for the linear, square, s. c. and b. c. c. lattices; z_2, z_3 and $v_{3,1}$ are given by $z_2=z(z-1)$, $z_3=z(z-1)^2$, and $v_{3,1}=z(z-1)(z-2)/2$. For the one-dimensional Heisenberg model, we have

$$\begin{aligned}
\langle s_0^z(0) s_0^z(t) \rangle &= \frac{1}{4} - \frac{t^2}{2!} J_{\perp}^2 + \frac{t^4}{4!} (9J_{\perp}^4 + 2J_{\perp}^2 J_{\parallel}^2) \\
&- \frac{t^6}{6!} (100J_{\perp}^6 + 55J_{\perp}^4 J_{\parallel}^2 + 8J_{\perp}^2 J_{\parallel}^4) \\
&+ \frac{t^8}{8!} (1225J_{\perp}^8 + 1232J_{\perp}^6 J_{\parallel}^2 + 420J_{\perp}^4 J_{\parallel}^4 + 32J_{\perp}^2 J_{\parallel}^6) \\
&- \frac{t^{10}}{10!} (15876J_{\perp}^{10} + 25704J_{\perp}^8 J_{\parallel}^2 + 16260J_{\perp}^6 J_{\parallel}^4 \\
&+ 2736J_{\perp}^4 J_{\parallel}^6 + 128J_{\perp}^2 J_{\parallel}^8) + O(t^{12}). \quad (4)
\end{aligned}$$

For $J_{//} = 0$, Eq. (4) is consistent with the result of the XY model obtained by Katsura, Horiguchi and Suzuki [6]. The t^4 term in Eq. (3) is consistent with McFadden and Tahir-Kheli's result [5]. McFadden and Tahir-Kheli's result [4] for the t^6 order is, however, not in agreement with the present result given in Eqs. (3) and (4). For $J_{\perp} = J_{//}$, Eq. (4) up to the t^8 term agree with the result of Nakamura [7].

The details of the calculation will be given in near future. In that work, the result for the two-time correlation functions of different spins will also be presented. The numerical calculation was carried out by using the computer NEAC 2200 of Computer Center, Tohoku University.

References

1. L. Van Hove, Phys. Rev. 95 (1954) 249; 95 (1954) 1374.
2. P. G. de Gennes, J. Phys. Chem. Solids 4 (1958) 223.
3. W. Marshall, in Critical Phenomena, ed. by M. S. Green and J. V. Sengers, National Bureau of Standards, (1966).
See also R. A. Tahir-Kheli and D. G. McFadden, Phys. Rev. 182 (1969) 604.
4. D. G. McFadden and R. A. Tahir-Kheli, Phys. Rev. to be published.
5. D. G. McFadden and R. A. Tahir-Kheli, Phys. Rev. to be published.
6. S. Katsura, T. Horiguchi and M. Suzuki, Physica 46 (1970) 67.
7. T. Nakamura, Lecture at the Institute for Solid State Physics, University of Tokyo, May, 1970.