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Statistical Mechanics of the *XY* Model. III*

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We continue the considerations of the first paper in this series by studying the time dependence of the spin-correlation functions in response to a step-function change in the external magnetic field. We find that these correlation functions exhibit nonergodic behavior.

I. INTRODUCTION

In a previous paper[1] we studied[2] time-dependent properties of the z-direction magnetization of the one-dimensional XY model. In particular, we considered an XY model in thermal equilibrium at temperature T in the presence of an external magnetic field H_1. At time $t=0$ the field is changed to some other value H_2, and $M_z(t)$ was computed. The most interesting aspect of $M_z(t)$ is that if $H_2=0$, then

$$\lim M_z(t) \neq 0 \quad \text{as } t\to\infty \; . \tag{1.1}$$

However, for all values of T, M_z is zero when the model is in thermal equilibrium. Therefore we concluded that (at least when $H_2=0$) the magnetization of this model does not exhibit ergodic behavior. This property was first discovered by Mazur[3] using results obtained by Niemeijer,[4] and further elaborated by Katsura, Horiguchi, and Suzuki.[5]

In this paper we continue the exploration of the nonergodic features of this system by examining the spin-correlation functions. After formulating the problem in Sec. II, we study, in Sec. III, the long-time behavior of $\rho_{zz}(R,t,T)$. We find that for any value of H_2,

$$\lim \rho_{zz}(R,t,T_1) \neq \rho_{zz}(R,0,T_2) \quad \text{as } t\to\infty \tag{1.2}$$

for any T_2. In other words the $t\to\infty$ limit of ρ_{zz} is not a correlation function of the XY model in thermal equilibrium. Furthermore, in Sec. IV, we study the limit

$$\lim_{R\to\infty}\lim_{t\to\infty}\rho_{xx}(R,t,T)$$

and find that the long-range order[2] exhibited by ρ_{xx} at $t=0$ totally disappears.

II. FORMULATION

Let c_i, $c_i^\dagger$ be the Fermi operators defined by (2.3) of I. Define the operators

$$A_i = c_i^\dagger + c_i \; , \tag{2.1}$$

$$B_i = c_i^\dagger - c_i \ . \qquad (2.2)$$

The expectation value

$$\langle A_i B_{i+R}\rangle = G_R \qquad (2.3)$$

is defined by (2.4) of II, and we find (2.15) of II to be

$$G_R = -\frac{1}{\pi}\int_0^\pi d\phi \cos\phi R \left(\frac{\tanh[\frac{1}{2}\beta\Lambda(a)]}{\Lambda(a)\,\Lambda^2(b)}\right)\{[\gamma^2 \sin^2\phi + (\cos\phi - a)(\cos\phi - b)](\cos\phi - b)$$
$$- (a-b)\gamma^2 \sin^2\phi \cos[2\Lambda(b)t]\} + \frac{\gamma}{\pi}\int_0^\pi d\phi \sin\phi R \sin\phi \left(\frac{\tanh[\frac{1}{2}\beta\Lambda(a)]}{\Lambda(a)\Lambda^2(b)}\right)$$
$$\{[\gamma^2 \sin^2\phi + (\cos\phi - a)(\cos\phi - b)] + (a-b)(\cos\phi - b)\cos[2\Lambda(b)t]\}, \qquad (2.4)$$

with

$$\Lambda(a) = [\gamma^2 \sin^2\phi + (a - \cos\phi)^2]^{1/2} \ . \qquad (2.5)$$

In an analogous way we define

$$\langle A_i A_{i+R}\rangle = \langle B_i B_{i+R}\rangle = S_R \ , \qquad (2.6)$$

and by the method of II we find

$$S_R = \frac{1}{N}\sum_p\left[-2\sin\left(\frac{2\pi p}{N}R\right)\langle a_p^\dagger a_p\rangle + 2\sin\left(\frac{2\pi p}{N}R\right)\mathrm{Re}\,[2\rho_{21}^p(t)]\right]. \qquad (2.7)$$

Using $\rho_{21}(t)$ given by (5.5) of I and passing to the thermodynamic limit, we obtain

$$S_R = \frac{\gamma(a-b)}{\pi}\int_0^\pi d\phi \sin\phi \sin\phi R\left(\frac{\sin[2t\Lambda(b)]}{\Lambda(a)\,\Lambda(b)}\right). \qquad (2.8)$$

In the equilibrium case S_R vanishes identically, and the Pfaffians ρ_{xx}, ρ_{yy} become Toeplitz determinants. However, this is not the case for finite t. For instance, by Wick's theorem we can express $\rho_{zz}(R, t, T)$ as

$$\rho_{zz}(R, T, t) = \langle A_j B_j A_{j+R} B_{j+R}\rangle$$
$$= \langle A_j B_j\rangle\langle A_{j+R} B_{j+R}\rangle - G_R G_{-R} - S_R S_{-R} \ . \qquad (2.9)$$

But because $\langle A_j B_j\rangle$ is the z-direction magnetization $m_z(t)$, studied in I, we obtain

$$\rho_{zz}(R, T, t) = m_z^2(t) - G_R(t)G_{-R}(t) - S_R(t)S_{-R}(t) \ . \qquad (2.10)$$

III. ASYMPTOTIC STUDY OF ρ_{zz}

In order to study the approach of $\rho_{zz}(t, R, T)$ to its infinite-time limit it is necessary to study the behavior of S_R and G_R for large t.

The limit $\rho_{zz}(\infty, R, T)$ can be obtained by the use of the Riemann-Lebesgue formula, and we find

$$\lim \rho_{zz}(t, R, T) = m_z^2(\infty) - G_R(\infty)G_{-R}(\infty) \quad \text{as } t\to\infty \ , \qquad (3.1)$$

where $G_R(\infty)$ is given by

$$G_R(\infty) = -\frac{1}{2\pi}\int_{-\pi}^{\pi} d\phi\, e^{-i\phi R}\,\frac{\tanh[\frac{1}{2}\beta\Lambda(a)]}{\Lambda(a)} \times \frac{[\gamma^2 \sin^2\phi + (\cos\phi - a)(\cos\phi - b)]}{[b - \cos\phi - i\gamma \sin\phi]} \qquad (3.2)$$

and $m_z(\infty)$ by (5.11) of I as

$$m_z(\infty) = \frac{1}{2\pi}\int_{-\pi}^{\pi} d\phi\, \frac{\tanh[\frac{1}{2}\beta\Lambda(a)]}{\Lambda(a)}\,\frac{(b - \cos\phi)}{\Lambda^2(b)} \times[\gamma^2 \sin^2\phi + (\cos\phi - b)] \ . \qquad (3.3)$$

By inspection it can be shown that ρ_{zz} does not approach its equilibrium limit (II, Sec. 3) even if one defines new "equilibrium temperature" $T_1(a)$ by the requirement that $m_z(\infty)$ be the equilibrium magnetization for this temperature.

The approach of the ground-state correlation $\rho_{zz}(t, R, 0)$ can be studied by setting $\beta = \infty$ in (2.10). As was the case for the asymptotic behavior of $m_z(t)$, we obtain a division into regions, dependent on whether $1 - \gamma^2 - b$ is greater, smaller, or equal to zero. Explicitly, by a similar method to I, Appendix B, we obtain

$$G_R \simeq G_R(\infty) + A_R + B_R \quad \text{as } t\to\infty \ , \qquad (3.4)$$

where A_R and B_R are given below for large t and fixed R. We also find

$$A_R \simeq \frac{1}{\pi}(a-b)\gamma^2(t\alpha)^{-1/2}\left\{\cos\left[2t\gamma\left(1 - \frac{b^2}{1-\gamma^2}\right)^{1/2} + \frac{\pi}{4}\right]\right\}\Gamma(\tfrac{1}{2})\left(1 - \frac{b^2}{(1-\gamma^2)^2}\right)^{1/2}\left\{\gamma^2\left[1 - \left(\frac{b}{1-\gamma^2}\right)^2\right]\right.$$
$$\left. + b^2\left(1 - \frac{1}{1-\gamma^2}\right)^2\right\}^{-1/2}\left\{\gamma^2\left[1 - \left(\frac{a}{1-\gamma^2}\right)^2\right]\right.$$

$$+\left(a-\frac{b}{1-\gamma^2}\right)^2\Bigg\}^{-1}\cos\left\{R\arctan\left[\left(\frac{1-\gamma^2}{b}\right)^2-1\right]^{1/2}\right\} \qquad \text{for } b<1-\gamma^2, \tag{3.5a}$$

$$A_R\sim(1/\pi)(a-b)\,\gamma^2\tfrac{1}{2}\Gamma(\tfrac{3}{4})(mt)^{-3/4}E_4(0)\cos[2t|b-1|+\tfrac{3}{8}\pi]\cos\pi R \qquad \text{for } b=1-\gamma^2, \tag{3.5b}$$

$$A_R\sim\frac{1}{\pi}(a-b)\,\gamma^2(2t)^{-3/2}\left[\left(\frac{|b-1|}{|b-(1-\gamma^2)|}\right)^{1/2}\Gamma(\tfrac{3}{2})E_1(|b-1|)\cos(2t|b-1|-\tfrac{1}{4}\pi)\right.$$

$$\left.+(-1)^R\left(\frac{|b-1|}{b+(1-\gamma^2)}\right)^{1/2}\Gamma(\tfrac{3}{2})E_1(|b+1|)\cos(2t|b+1|+\tfrac{1}{4}\pi)\right] \qquad \text{for } b>1-\gamma^2. \tag{3.5c}$$

Note that A_R has very similar asymptotic behavior to $m_z(t)$ given by (5.13)–(5.15) of I. The constants α, m, E_j are defined in I, Appendix B. The results of B_R are given as

$$B_R\simeq\frac{\gamma(a-b)R}{\pi}(2t)^{-3/2}\Gamma(\tfrac{3}{2})\left[-|1-b|E_1(|b-1|)\left(\frac{|b-1|}{|b-(1-\gamma^2)|}\right)^{1/2}\cos(2t|b-1|-\tfrac{1}{4}\pi)\right.$$

$$\left.-(-1)^R|b+1|\left(\frac{|b+1|}{|b+(1-\gamma^2)|}\right)^{1/2}E_1(|b+1|)\cos(2t|b+1|+\tfrac{1}{4}\pi)\right] \qquad \text{for } b>1-\gamma^2, \tag{3.6a}$$

$$B_R\simeq[\gamma^3(a-b)R/\pi]\tfrac{1}{2}\Gamma(\tfrac{3}{4})(mt)^{-3/4}E_4(0)\cos(\pi R)\cos(2t|b-1|+\tfrac{3}{2}\pi) \qquad \text{for } b=1-\gamma^2, \tag{3.6b}$$

$$B_R\simeq\frac{\gamma^3(a-b)R}{\pi(1-\gamma^2)}(t\alpha)^{-1/2}\Gamma(\tfrac{1}{2})\cos\left\{(R-1)\arctan\left[\left(\frac{1-\gamma^2}{b}\right)^2-1\right]^{1/2}\right\}\left[1-\left(\frac{b}{1-\gamma^2}\right)^2\right]^{1/2}$$

$$\times\left\{\gamma^2\left[1-\left(\frac{b}{1-\gamma^2}\right)^2\right]+b^2\left(1-\frac{1}{1-\gamma^2}\right)^2\right\}^{-1/2}\left\{\gamma^2\left[1-\left(\frac{b}{1-\gamma^2}\right)^2\right]\right.$$

$$\left.+\left(a-\frac{b}{1-\gamma^2}\right)^2\right\}^{-1}\cos\left\{\left[2\gamma t\left(1-\frac{b^2}{1-\gamma^2}\right)^{1/2}\right]+\frac{\pi}{4}\right\} \qquad \text{for } b<1-\gamma^2. \tag{3.6c}$$

We see that B_R has similar properties to A_R for t large. By the same method, we find S_R to have the same behavior for large t. To show that similarity we give S_R for $b<1-\gamma^2$ as

$$S_R\cong\frac{R\gamma(a-b)}{\pi}\cos\left\{(R-1)\arctan\left[\left(\frac{1-\gamma^2}{b^2}\right)^2-1\right]^{1/2}\right\}\cos\left[\frac{\pi}{4}+2\gamma t\left(1-\frac{b^2}{1-\gamma^2}\right)^{1/2}\right]$$

$$\times\Gamma(\tfrac{1}{2})(t\alpha)^{-1/2}\left\{\gamma^2\left[1-\left(\frac{b}{1-\gamma^2}\right)^2\right]+\left(a-\frac{b}{1-\gamma^2}\right)^2\right\}^{-1/2}\left\{\gamma^2\left[1-\left(\frac{b}{1-\gamma^2}\right)^2\right]+b\left[1-\frac{1}{1-\gamma^2}\right]^2\right\}^{-1/2}. \tag{3.7}$$

Furthermore, for $b=1-\gamma^2$, we find $S_R=O(t^{-3/4})$, and for $b>1-\gamma^2$, we find $S_R=O(t^{-3/2})$. Hence, it is clear the term S_RS_{-R} does not contribute to the leading term of the asymptotic expansion of ρ_{zz}, which is given as (leading term)

$$\rho_{zz}\simeq\rho_{zz}(\infty)+G_{-R}(\infty)(A_R+B_R)+G_R(\infty)(A_{-R}+B_{-R}) \qquad \text{as } t\to\infty, \tag{3.8}$$

where A_R, B_R are given by (3.5) and (3.6) and $G_R(\infty)$ by (3.2).

We conclude this section with the remark that the zz correlation function approaches its nonergodic limit in the same fashion as $m_z(t)$ approaches its limit.

IV. TRANSVERSE CORRELATIONS

In this section we deal with ρ_{xx} for the ground state. A long-range order was found in II, and the nonergodicity of ρ_{xx} expresses itself in destruction of this long-range order.

We take the infinite-time limit, in which S_R vanishes and $G_R(t)$ becomes $G_R(\infty)$. At the ground state we have

$$G_R(\infty)=-\frac{1}{2\pi}\int_{-\pi}^{\pi}d\phi\,e^{-i\phi R}\times\frac{[\gamma^2\sin^2\phi+(\cos\phi-a)(\cos\phi-b)]}{[\gamma^2\sin^2\phi+(\cos\phi-a)^2]^{1/2}(b-\cos\phi-i\gamma\sin\phi)}. \tag{4.1}$$

In order to evaluate ρ_{xx} we substitute $G_R(\infty)$ in (2.8a) of II and use Szëgo's theorem. It takes some algebra to show that $k_0 \neq 0$, where k_0 is explicitly given as

$$k_0 = \frac{1}{2\pi}\int_{-\pi}^{\pi} d\phi \times \ln\left(\frac{\gamma^2 \sin^2\phi + (\cos\phi - a)(\cos\phi - b)}{[\gamma^2\sin^2\phi + (\cos\phi - a)^2]^{1/2}(b - \cos\phi - i\gamma\sin\phi)}\right). \quad (4.2)$$

This means that ρ_{xx} decays exponentially rapidly to zero and the nonergodic nature of ρ_{xx} manifests itself in a qualitative manner.

We wish to study the approach to ρ_{xx} to its limit. Unfortunately, we are unable to do this in a rigorous manner, since we cannot analyze the resulting block Toeplitz determinant, whose generating matrix is given by

$$C_R = \frac{1}{2\pi}\int_{-\pi}^{\pi} e^{-i\phi R}\begin{bmatrix} \sigma_\gamma & g_\gamma \\ -g_{-\gamma} & \sigma_\gamma \end{bmatrix}, \quad (4.3)$$

where σ_γ, g_γ are given by

$$\sigma_\gamma = i(a-b)\gamma\sin\phi\sin[2t\Lambda(a)]/\Lambda(a)\Lambda(b), \quad (4.4)$$

$$g_\gamma = -[\Lambda(a)\Lambda^2(b)]^{-1}(\{[\gamma^2\sin^2\phi + (\cos\phi - a)(\cos\phi - b)](\cos\phi - b) - (a-b)\gamma^2\sin^2\phi\cos[2\Lambda(b)t]\} - i\gamma\sin\phi\{[\gamma^2\sin^2\phi + (\cos\phi - a)(\cos\phi - b)] + (a-b)(\cos\phi - b)\cos[2\Lambda(b)t]\}) . \quad (4.5)$$

The expression for g_γ can be somewhat simplified as

$$g_\gamma = -\frac{\gamma^2\sin^2\phi + (\cos\phi - a)(\cos\phi - b)}{[\gamma^2\sin^2\phi + (\cos\phi - a)^2]^{1/2}(b - \cos\phi - i\gamma\sin\phi)} - \frac{(a-b)\cos[2\Lambda(b)t]\, i\gamma\sin\phi}{\Lambda(a)(b - \cos\phi - i\gamma\sin\phi)} . \quad (4.6)$$

Because of the relation between cyclic and Toeplitz matrices we believe that the generalization of Szëgo's theorem yields

$$U\exp\left(\frac{R}{2\pi}\int_{-\pi}^{\pi} d\phi\, \ln|[\sigma_\gamma^2(\phi) + g_\gamma(\phi)g_{-\gamma}(\phi)]|\right) \quad \text{as } t, R \to \infty , \quad (4.7)$$

where U is a positive constant we are unable to compute. Expression (4.7) can be written explicitly as

$$\rho_{xx} \simeq U\exp\left\{\frac{R}{2\pi}\int_{-\pi}^{\pi} d\phi\, \ln\left[\left(\frac{\Lambda(b)}{\Lambda(a)}\right)^2 - \frac{2(\cos\phi - b)(a-b)}{\Lambda(a)} + \frac{(a-b)^2\gamma^2\sin^2\phi\cos 4\Lambda(b)t}{\Lambda^2(a)\Lambda^2(b)}\right]\right\}. \quad (4.8)$$

We make the specialization that $a - b$ is very small, and expand the log function in powers of $a - b$:

$$\rho_{xx} \simeq U\exp\left\{\frac{R}{2\pi}\int_{-\pi}^{\pi} d\phi\left[\ln\left(\frac{\Lambda^2(b)}{\Lambda^2(a)} - \frac{2(a-b)(\cos\phi - b)}{\Lambda(a)}\right) + \frac{(a-b)^2\gamma^2\sin^2\phi\cos 4\Lambda(b)t}{\Lambda^4(b)}\right]\right\} .$$

We observe that the time-dependent part of the exponential is very similar to $m_z(t)$. In particular, the approach of ρ_{xx} to its $t \to \infty$ limit will be some oscillatory factor times $t^{-3/2}$ if $b > 1 - \gamma^2$, $t^{-3/4}$ if $b = 1 - \gamma^2$, and $t^{-1/2}$ if $b < 1 - \gamma^2$.

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