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Spin Correlation Functions of the X-Y Model

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We consider the one-dimensional X-Y model of Lieb, Schulz, and Mattis and study the asymptotic behavior of each of the three correlation functions $\langle\sigma_0{}^i\sigma_N{}^i\rangle=\rho_N{}^i$, where $i=x$, y, or z. We study in detail the influence of X-Y anisotropy by separately studying the correlation functions in both the isotropic and anisotropic cases at both nonzero and zero temperatures. For nonzero temperature we derive both low- and high-temperature expansions for all three correlations and show that these correlations go to zero exponentially as $N\to\infty$. The behavior near $T=0$ is studied in the isotropic case by considering the $N\to\infty$ limit with TN fixed, while in the anisotropic case we must hold T^2N fixed as $N\to\infty$. In this manner we obtain the $T=0$ result that if the interaction is stronger in the x direction, then $\rho_N{}^x$ approaches a constant exponentially while $\rho_N{}^y$ approaches zero exponentially as $N\to\infty$. We finally show that in the isotropic case at $T=0$ that $\rho_N{}^x=\rho_N{}^y\to N^{-1/2}$. In all cases, at least the first two terms of the asymptotic series are explicitly given.

1. INTRODUCTION

THE X-Y model of Lieb, Schulz, and Mattis[1] is a system of $\mathfrak{N}$ spin-$\frac{1}{2}$ particles fixed on a line with nearest-neighbor interactions given by the Hamiltonian

$$H=-\sum(\sigma_j{}^x\sigma_{j+1}{}^x+\alpha\sigma_j{}^y\sigma_{j+1}{}^y), \qquad (1.1)$$

where

$$\sigma_j{}^x=\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}, \quad \sigma_j{}^y=\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix}, \quad \sigma_j{}^z=\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}$$

are the Pauli matrices. When $\alpha=0$ this model reduces to the Ising model, whereas when $\alpha=1$ the interaction is isotropic in the X-Y plane and is a special case of the anisotropic Heisenberg model. One reason that LSM introduced this model was to study the effect which the presence or absence of isotropy has on the three correlation functions

$$\rho_N{}^i=\langle\sigma_0{}^i\sigma_N{}^i\rangle, \qquad (1.2)$$

where i may be x, y, or z. These authors found that $\rho_N{}^z$ could be expressed as the product of two integrals and that $\rho_N{}^x$ and $\rho_N{}^y$ could be expressed as the product of two large Toeplitz determinants. They furthermore found several bounds on these correlation functions as $N\to\infty$ which establish a distinct difference between the isotropic and anisotropic cases. However, except for $\rho_N{}^z$ at $T=0$ and $\alpha=1$ the explicit asymptotic behavior of the correlation functions was not obtained. It is the purpose of this paper to characterize the differences between the isotropic and anisotropic cases in as much detail as possible by explicitly evaluating the asymptotic behavior as $N\to\infty$ of all three correlation functions both in the ground state and at nonzero temperatures.

The correlation function $\rho_N{}^z$ is studied in Sec. 2 where we consider the cases (a) $\alpha=1$ or $\neq1$ for $T>0$ fixed and $N\to\infty$, (b) $\alpha\neq1$ and T^2N fixed as $N\to\infty$, and (c) $\alpha=1$ and TN fixed as $N\to\infty$. It is necessary to consider these last two cases in order to recover the ground-state correlation functions from the nonzero-temperature results.

The correlation function $\rho_N{}^x$ is studied in Sec. 3 by using a theorem of Szego[2] to asymptotically evaluate the Toeplitz determinants. This yields the leading term in the asymptotic expansion of $\rho_N{}^x$. When $T>0$, $\rho_N{}^x$ goes to zero as $N\to\infty$. A high-temperature expansion is given by (3.15) and a low-temperature expansion for $\alpha<1$ by (3.35). When $T=0$, $\rho_N{}^x$ has the limit $(1-\alpha^2)^{1/2}$ as $N\to\infty$ [Eq. (3.36)].

In Sec. 4, we study $\rho_N{}^y$ for $\alpha<1$ by using some recent results of Wu.[3] For $T>0$ and $N\to\infty$, we obtain a high-temperature expansion [Eq. (4.19)] and a low-temperature expansion [Eq. (4.23)]. We also study the approach to the ground state by studying the $N\to\infty$ limit with T^2N held fixed. In the ground state, we find [Eq. (4.28)] that $\rho_N{}^y$ approaches zero exponentially as $N\to\infty$.

In Sec. 5, we return to $\rho_N{}^x$ and study its behavior for T^2N fixed and $N\to\infty$ by computing the first correction term to the result of Sec. 3. We are then able to see that at $T=0$, $\rho_N{}^x$ approaches its limiting value exponentially rapidly [Eq. (5.15)]. Finally, we study $\rho_N{}^x=\rho_N{}^y$ in the isotropic case. When $T>0$, we obtain a low-temperature asymptotic expansion [Eq. (6.8)]. In the ground state, the Toeplitz determinants may be exactly evaluated and we find that $\rho_N{}^x$ approaches zero as $N^{-1/2}$ when $N\to\infty$. In contrast to all other correlation functions of

[1] E. Lieb, T. Schultz, and D. Mattis, Ann. Phys. (N.Y.) **16**, 407 (1961). This paper will henceforth be referred to as LSM. Our Hamiltonian differs from these authors in several minor details. Our α is related to their γ by $\alpha=(1-\gamma)(1+\gamma)^{-1}$ and we obtain our Hamiltonian by multiplying theirs by $-4(1+\gamma)^{-1}$. We have chosen to treat the ferromagnetic case and use Pauli matrices instead of the matrices $\mathbf{s}=\frac{1}{2}\boldsymbol{\sigma}$. For recent related work, see also Th. Niemeyer, Physica **36**, 377 (1967).

[2] V. Grenander and G. Szego, *Toeplitz Forms and Their Applications* (University of California Press, Berkeley, 1958). See also E. W. Montroll, R. B. Potts, and J. C. Ward, J. Math. Phys. **4**, 308 (1963).

[3] T. T. Wu, Phys. Rev. **149**, 380 (1966). Equations from this paper will be referred to by a w after the equation or section number.

the X-Y model, this approach of $\rho_N{}^y$ to its $N\rightarrow\infty$ limit is not an integrable function of N. This implies that at $T=0$ when $H_x(H_y)$ is near zero that the $x(y)$ component of the magnetization behaves as

$$M_x\sim \operatorname{sgn}(H_x)K\,|\,H_x\,|^{1/3}. \tag{1.3}$$

2. CORRELATION $\rho_N{}^z$

It has been shown by LSM[1] that if we impose periodic boundary conditions on (1.1) and take the thermodynamic limit, the correlation function $\rho_N{}^z$ for $N\neq 0$ is given by

$$\begin{aligned}\rho_N{}^z&=-G_NG_{-N} && \text{if } N \text{ is odd}\\ &=0 && \text{if } N \text{ is even,}\end{aligned} \tag{2.1}$$

where

$$\begin{aligned}G_n&=-(1+\alpha)^{-1}[L_{n+1}+\alpha L_{n-1}] && \text{if } n \text{ is odd}\\ &=0 && \text{if } n \text{ is even,}\end{aligned} \tag{2.2}$$

$$L_n=-(2/\pi)\int_0^{\pi/2}d\theta\,[1-4\alpha(1+\alpha)^{-2}\sin^2\theta]^{-1/2}\cos n\theta \times\tanh\{\beta(1+\alpha)[1-4\alpha(1+\alpha)^{-2}\sin^2\theta]^{1/2}\}, \tag{2.3}$$

and $\beta=(kT)^{-1}$. This is conveniently rewritten as

$$G_{2n-1}(\alpha) =(-1)^n(2\pi)^{-1}\int_0^{2\pi}d\phi\; e^{in\phi}[(1-\alpha e^{-i\phi})/(1-\alpha e^{i\phi})]^{1/2} \times\tanh\{\beta[(1-\alpha e^{i\phi})(1-\alpha e^{-i\phi})]^{1/2}\}, \tag{2.4}$$

where the square roots are defined positive at $\phi=\pi$. It is easily seen that

$$G_{-(2n-1)}(\alpha)=G_{2n-1}(\alpha^{-1}), \tag{2.5}$$

so that

$$\rho_{2n-1}{}^z(\alpha)=-G_{2n-1}(\alpha)G_{2n-1}(\alpha^{-1}). \tag{2.6}$$

Unless $\beta=\infty$, the integrand of (2.4) consists of an infinite number of poles on the real $e^{i\phi}$ axis. We make this manifest by using the partial-fraction decomposition of tanh$z$ to write

$$[(1-\alpha e^{-i\phi})/(1-\alpha e^{i\phi})]^{1/2} \times\tanh\{\beta[(1-\alpha e^{i\phi})(1-\alpha e^{-i\phi})]^{1/2}\}=2\beta(1-\alpha e^{-i\phi}) \times\sum_{m=1}^{\infty}[\beta^2(1-\alpha e^{i\phi})(1-\alpha e^{-i\phi})+\tfrac{1}{4}\pi^2(2m-1)^2]^{-1}. \tag{2.7}$$

Define ξ_m to be that solution of

$$\beta^2(1-\alpha\xi_m)(1-\alpha\xi_m{}^{-1})+\tfrac{1}{4}\pi^2m^2=0 \tag{2.8}$$

which obeys $|\,\xi_m\,|\leq 1$. Explicitly,

$$\xi_m{}^{\pm1}=\tfrac{1}{2}\alpha^{-1}\{1+\alpha^2+(\tfrac{1}{2}\beta^{-1}\pi m)^2\mp[((1-\alpha)^2+(\tfrac{1}{2}\beta^{-1}\pi m)^2) \times((1+\alpha)^2+(\tfrac{1}{2}\beta^{-1}\pi m)^2)]^{1/2}\}, \tag{2.9}$$

where for positive m the square root is defined positive. Evaluating (2.4) by residues we find for $n\geq 1$ and all α and β that

$$G_{2n-1}(\alpha)=(-1)^{n+1}2\beta^{-1} \times\sum_{m=1}^{\infty}\xi_{2m-1}{}^{n-1}(1-\alpha^{-1}\xi_{2m-1})(\xi_{2m-1}{}^{-1}-\xi_{2m-1})^{-1}. \tag{2.10}$$

We wish to make explicit the asymptotic behavior of $\rho_N{}^z$ as $N\rightarrow\infty$ for those ranges of T and α where we will also obtain asymptotic expansions of $\rho_N{}^x$ and $\rho_N{}^y$. We therefore consider the three special cases mentioned in the Introduction.

A. $T\neq 0$ and $N>\infty$ for All α

When n is sufficiently large and $T\neq 0$ all terms in (2.10) are exponentially small compared with the first, so that $\rho_{2n-1}{}^z$ is asymptotically given as

$$\rho_{2n-1}{}^z\sim-4\beta^{-2}[\xi_1(\alpha)^{1/2}\xi_1(\alpha^{-1})^{1/2}]^{2n-1}[\xi_1(\alpha)^{-1/2}\alpha^{1/2}-\xi_1(\alpha)^{1/2}\alpha^{-1/2}][\xi_1(\alpha^{-1})^{-1/2}\alpha^{-1/2}-\xi_1(\alpha^{-1})^{1/2}\alpha^{1/2}] \times[\xi_1(\alpha)^{-1}-\xi_1(\alpha)]^{-1}[\xi_1(\alpha^{-1})^{-1}-\xi_1(\alpha^{-1})]^{-1}. \tag{2.11}$$

When T is large, we may further expand ξ_m as

$$\xi_m=\alpha(2\beta/\pi m)^2[1-(2\beta/\pi m)^2(1+\alpha^2)+(2\beta/\pi m)^4(1+3\alpha^2+\alpha^4)+O(\beta^6)] \tag{2.12}$$

to find for all α

$$\rho_{2n-1}{}^z(\alpha)\sim-16\pi^{-1}\{(2\beta/\pi)^2[1-\tfrac{1}{2}(2\beta/\pi)^2(\alpha^{-1}+\alpha)^2+O(\beta^4)]\}^{2n-1}[1-\tfrac{1}{2}(2\beta/\pi)^2(\alpha^{-2}+6+\alpha^2)+O(\beta^4)]. \tag{2.13}$$

If T is small and $\alpha\neq 1$ we may use the expansion

$$\xi_m{}^{\pm1}=\tfrac{1}{2}\alpha^{-1}\{1+\alpha^2+(\tfrac{1}{2}\beta^{-1}\pi m)^2\mp\,|\,1-\alpha^2\,|\,[1+(\tfrac{1}{2}\beta^{-1}\pi m)^2(1+\alpha^2)(1-\alpha^2)^{-2}-2\alpha^2(\tfrac{1}{2}\beta^{-1}\pi m)^4(1-\alpha^2)^{-4}+O(\beta^{-6})]\} \tag{2.14}$$

to obtain

$$\rho_{2n-1}{}^z(\alpha)\sim-\beta^{-4}\pi^2\{\alpha[1-\tfrac{1}{2}(\tfrac{1}{2}\beta^{-1}\pi)^2(1+\alpha^2)(1-\alpha^2)^{-1}+O(\beta^{-4})]\}^{2n-1}\alpha^{-1}(\alpha^{-1}-\alpha)^{-2} \times[1-\tfrac{1}{2}\beta^{-2}\pi^2(1+\alpha^2)(3+\alpha^2)(1-\alpha^2)^{-2}+O(\beta^{-4})]. \tag{2.15}$$

If T is small and $\alpha=1$ we correspondingly find

$$\rho_{2n-1}{}^z(1)=-\beta^{-2}[1-\tfrac{1}{2}\beta^{-1}\pi+\tfrac{1}{2}(\tfrac{1}{2}\beta^{-1}\pi)^2+O(\beta^{-3})]^{2n-1}[1-\tfrac{1}{4}(\tfrac{1}{2}\beta^{-1}\pi)^2+O(\beta^{-4})]. \tag{2.16}$$

B. $\alpha<1$, T^2N Fixed and $N\to\infty$

The expansions (2.15) and (2.16) are valid only when n is so large that only the first term of (2.10) contributes significantly. This restriction prevents us from setting $\beta=\infty$ in (2.15) and (2.16). When $\alpha<1$ we may study the approach of $\rho_{2n-1}{}^z$ to its ground-state value by defining

$$q_< = (2n-1)\beta^{-2}\tfrac{1}{8}(1-\alpha^2)^{-1} \qquad (2.17)$$

and considering the $n\to\infty$ limit with $q_<$ fixed. We may then recover the ground-state correlation function by setting $q_<=0$. We first expand $G_{2n-1}(\alpha)$ by writing

$$\xi_m{}^{n-1/2}=\alpha^{n-1/2}\exp(-q_<\pi^2m^2) \times[1+\pi^4q_<{}^2(2n-1)^{-1}(1-\alpha^2)^{-1}(1+\alpha^2)m^4 +O((2n-1)^{-2}m^6)]. \qquad (2.18)$$

This expansion breaks down when $q_<m^2\sim(2n-1)^{1/2}$, but when m^2 is this large, $\xi_m{}^{n-1/2}$ is exponentially smaller than $\xi_1{}^{n-1/2}$ and does not contribute asymptotically. Therefore, we use (2.18) in (2.10) to find

$$G_{2n-1}(\alpha)\sim(-1)^n\alpha^n 8\sqrt{2}(1-\alpha^2)^{-1/2}q_<{}^{3/2}(2n-1)^{-3/2} \times\left[\frac{\partial}{\partial q_<}+(2n-1)^{-1}(1-\alpha^2)^{-1}(1+\alpha^2) \times\left(3q_<\frac{\partial^2}{\partial q_<{}^2}+q_<{}^2\frac{\partial^3}{\partial q_<{}^3}\right)\right]\sum_{m=1}^{\infty}\exp[-q_<\pi^2(2m-1)^2], \qquad (2.19)$$

where the derivatives in the bracket all act on the infinite series. This series may be expressed as an elliptic θ function of the third kind.[4] However, for the purpose of studying the behavior of G_{2n-1} near $q_<=0$ we need only use the Poisson summation formula to write

$$\sum_{m=1}^{\infty}\exp[-q_<\pi^2(2m-1)^2] =\tfrac{1}{4}(\pi q_<)^{-1/2}[1+2\sum_{m=1}^{\infty}(-1)^m\exp(-m^2/4q_<)]. \qquad (2.20)$$

Therefore,

$$G_{2n-1}(\alpha)\sim(-1)^{n+1}\alpha^n(1-\alpha^2)^{-1/2}(2/\pi)^{1/2}(2n-1)^{-3/2}\{1+2\sum_{m=1}^{\infty}(-1)^m\exp(-m^2/4q_<)(1-m^2/2q_<) -\tfrac{1}{4}(2n-1)^{-1}(1-\alpha^2)^{-1}(1+\alpha^2)[3+2\sum_{m=1}^{\infty}(-1)^m\exp(-m^2/4q_<) \times[3+9(m^2/2q_<)-9(m^2/2q_<)^2+(m^2/2q_<)^3]]+O((2n-1)^{-2})\}. \qquad (2.21)$$

We expand $G_{2n-1}(\alpha^{-1})$ similarly by defining

$$q_> = (2n-1)\beta^{-2}\tfrac{1}{8}(\alpha^{-2}-1)^{-1}=\alpha^2q_< \qquad (2.22)$$

and using

$$\xi_m(\alpha^{-1})^{n-1/2}\sim\alpha^{n-1/2}\exp(-q_>m^2)[1+q_>{}^2(2n-1)^{-1}(1-\alpha^2)^{-1}(1+\alpha^2)m^4+O((2n-1)^{-2}m^6)] \qquad (2.23)$$

to find

$$G_{2n-1}(\alpha^{-1})\sim(-1)^{n+1}\alpha^n4\sqrt{2}(\alpha^{-2}-1)^{1/2}q_>{}^{1/2}(2n-1)^{-1/2} \times\{1+(2n-1)^{-1}(1-\alpha^2)^{-1}(1+\alpha^2)[q_>\partial/\partial q_>+q_>{}^2\partial^2/\partial q_>{}^2]\}\sum_{m=0}^{\infty}\exp[-q_>\pi^2(2m+1)^2]$$
$$=(-1)^{n+1}\alpha^{n-1}(1-\alpha^2)^{1/2}(2/\pi)^{1/2}(2n-1)^{-1/2}\{1+2\sum_{m=1}^{\infty}(-1)^m\exp(-m^2/4q_>)+\tfrac{1}{4}(2n-1)^{-1}(1-\alpha^2)^{-1}(1+\alpha^2) \times[1+2\sum_{m=1}^{\infty}(-1)^m\exp(-m^2/4q_>)(1-4(m^2/2q_>)+(m^2/2q_>)^2)]+O((2n-1)^{-2})\}. \qquad (2.24)$$

We finally may use (2.21) and (2.24) in (2.6) to find

$$\rho_{2n-1}{}^z\sim-\alpha^{2n-1}2\pi^{-1}(2n-1)^{-2}\{[1+2\sum_{m=1}^{\infty}(-1)^m\exp(-m^2/4q_<)(1-m^2/2q_<)][1+2\sum_{m=1}^{\infty}(-1)^m\exp(-m^2/4q_>)]$$
$$+\tfrac{1}{4}(2n-1)^{-1}(1-\alpha^2)^{-1}(1+\alpha^2)[[1+2\sum_{m=1}^{\infty}(-1)^m\exp(-m^2/4q_<)(1-m^2/2q_<)] \times[1+2\sum_{m=1}^{\infty}(-1)^m\exp(-m^2/4q_>)(1-4(m^2/2q_>)+(m^2/2q_>)^2)]-[1+2\sum_{m=1}^{\infty}(-1)^m\exp(-m^2/4q_>)]$$
$$\times[3+2\sum_{m=1}^{\infty}(-1)^m\exp(-m^2/4q_<)(3+9(m^2/2q_<)-9(m^2/2q_<)^2+(m^2/2q_<)^3)]]+O((2n-1)^{-3})\}. \qquad (2.25)$$

[4] Bateman Manuscript Project, *Higher Transcendental Functions*, edited by A. Erdelyi (McGraw-Hill Book Co., New York, 1953), Vol. 2, p. 355.

This is the desired answer. We note in particular that as $q_>$ goes to zero, (2.25) approaches its $q_>=0$ value *exponentially* rapidly. This $T=0$ correlation function is

$$\rho_{2n-1}^z \sim -\alpha^{2n-1}2\pi^{-1}(2n-1)^{-2} \times[1-\tfrac{1}{2}(2n-1)^{-1}(1-\alpha^2)^{-1}(1+\alpha^2)+O((2n-1)^{-2})]. \tag{2.26}$$

This asymptotic expansion improves on the previous result of LSM who show that ρ_{2n-1}^z is bounded by a constant times $(2n-1)^{-4}$.

C. $\alpha=1$, TN Fixed, and $N\to\infty$

When $\alpha=1$ we may study the approach of ρ_{2n-1}^z to its ground-state value in a manner similar to the $\alpha<1$ case. The principal difference is that we must expand in terms of the parameter

$$q=\tfrac{1}{4}(2n-1)\beta^{-1}\pi. \tag{2.27}$$

We use the expansion

$$\xi_m(1)^{n-1/2}=e^{-qm}[1+\tfrac{1}{6}q^3(2n-1)^{-2}m^3+O((2n-1)^{-3}m^4)] \tag{2.28}$$

in (2.10) to find

$$\rho_{2n-1}^z(1)\sim -16q^2\pi^{-2}(2n-1)^{-2}(e^q-e^{-q})^{-2} \times\{1-\tfrac{1}{6}(2n-1)^{-2}[3q^2(e^q-e^{-q})^{-2} \times[2(e^q+e^{-q})^2-(e^q-e^{-q})^2]-q^3(e^q-e^{-q})^{-3}(e^q+e^{-q}) \times[6(e^q+e^{-q})^2-5(e^q-e^{-q})^2]]+\cdots\}. \tag{2.29}$$

This is the desired answer. We may now let $q\to 0$ and recover the asymptotic expansion of the ground-state correlation function

$$\rho_{2n-1}^z(1)\sim -4\pi^{-2}(2n-1)^{-2}. \tag{2.30}$$

This derivation is only valid asymptotically. However, if we set $T=0$ directly in (2.4) we see, as first noted by LSM, that (2.30) holds as an equality for all n.

3. CORRELATION ρ_N^x

It has been shown by LSM that if we define the $n\times n$ Toeplitz determinant

$$R_n=\begin{vmatrix} G_{-1} & G_{-3} & \cdots & G_{-2n+1} \\ G_1 & G_{-1} & \cdots & G_{-2n+3} \\ \cdot & \cdot & \cdots & \cdot \\ \cdot & \cdot & \cdots & \cdot \\ \cdot & \cdot & \cdots & \cdot \\ G_{2n-3} & G_{2n-5} & \cdots & G_{-1} \end{vmatrix}, \tag{3.1}$$

then for $N\geq 1$

$$\begin{aligned} \rho_N^x(\alpha) &= \rho_{2n-1}^x(\alpha)=R_{n-1}R_n && \text{if } N \text{ is odd,} \\ &= \rho_{2n}^x(\alpha)=R_n^2 && \text{if } N \text{ is even} \end{aligned} \tag{3.2}$$

and

$$\rho_N^y(\alpha)=\rho_N^x(\alpha^{-1}). \tag{3.3}$$

In this section, we compute the asymptotic behavior of ρ_N^x when $N\to\infty$ and T is fixed by a direct application of Szego's theorem.[2] It is convenient to multiply all odd-numbered rows and columns by -1 and to transpose the resulting determinant. We define

$$a_n=(-1)^nG_{-2n-1} =(2\pi)^{-1}\int_0^{2\pi} d\phi\, e^{-in\phi}[(1-\alpha e^{-i\phi})/(1-\alpha e^{i\phi})]^{1/2} \times \tanh\{\beta[(1-\alpha e^{i\phi})(1-\alpha e^{-i\phi})]^{1/2}\} \tag{3.4}$$

to obtain

$$R_n=\begin{vmatrix} a_0 & a_{-1} & \cdots & a_{-n+1} \\ a_1 & a_0 & \cdots & a_{-n+2} \\ \cdot & \cdot & \cdots & \cdot \\ \cdot & \cdot & \cdots & \cdot \\ \cdot & \cdot & \cdots & \cdot \\ a_{n-1} & a_{n-2} & \cdots & a_0 \end{vmatrix}. \tag{3.5}$$

We may immediately apply Szego's theorem to the determinant (3.5) when $\alpha<1$. This gives as $n\to\infty$

$$R_n\sim G^n \exp\left(\sum_{m=1}^{\infty} mk_mk_{-m}\right), \tag{3.6}$$

where

$$G=\exp(2\pi)^{-1}\int_{-\pi}^{\pi} d\phi \ln\{[(1-\alpha e^{-i\phi})/(1-\alpha e^{i\phi})]^{1/2} \times \tanh[\beta((1-\alpha e^{i\phi})(1-\alpha e^{-i\phi}))^{1/2}]\} \tag{3.7}$$

and

$$\sum_{m=-\infty}^{\infty} k_m e^{im\phi}=\ln\{[(1-\alpha e^{-i\phi})/(1-\alpha e^{i\phi})]^{1/2} \times \tanh[\beta((1-\alpha e^{i\phi})(1-\alpha e^{-i\phi}))^{1/2}]\}. \tag{3.8}$$

We may obtain a more explicit evaluation of G if we use the infinite-product representation of the hyperbolic tangent to write

$$[(1-\alpha e^{-i\phi})/(1-\alpha e^{i\phi})]^{1/2}\tanh\{\beta[(1-\alpha e^{i\phi})(1-\alpha e^{-i\phi})]^{1/2}\}=\beta(1-\alpha e^{-i\phi}) \times\prod_{m=1}^{\infty}[(2\beta\pi^{-1})^2(2m)^{-2}\alpha\xi_{2m}^{-1}(e^{i\phi}-\xi_{2m})(e^{-i\phi}-\xi_{2m})] \Big/ \prod_{m=1}^{\infty}[(2\beta\pi^{-1})^2(2m-1)^{-2}\alpha\xi_{2m-1}^{-1}(e^{i\phi}-\xi_{2m-1})(e^{-i\phi}-\xi_{2m-1})], \tag{3.9}$$

where we have used the definition of ξ_m [Eq. (2.8)]. Using this expansion in the integral of (3.7) we find that

$$G=\beta\prod_{m=1}^{\infty}[(2\beta\pi^{-1})^2(2m)^{-2}\alpha\xi_{2m}^{-1}] \Big/ \prod_{m=1}^{\infty}[(2\beta\pi^{-1})^2(2m-1)^{-2}\alpha\xi_{2m-1}^{-1}]. \tag{3.10}$$

We may also use (3.9) to obtain an explicit formula for k_m by first rewriting (3.8) as

$$\sum_{m=-\infty}^{\infty} k_m e^{im\phi} = \ln\beta + \sum_{m=1}^{\infty} \{\ln[(2\beta\pi^{-1})^{-2}(2m-1)^2\alpha^{-1}\xi_{2m-1}] - \ln[(2\beta\pi^{-1})^{-2}(2m)^2\alpha^{-1}\xi_{2m}]\} + \ln(1-\alpha e^{-i\phi})$$
$$+\sum_{m=1}^{\infty} \ln[(1-\xi_{2m}e^{i\phi})(1-\xi_{2m}e^{-i\phi})(1-\xi_{2m-1}e^{i\phi})^{-1}(1-\xi_{2m-1}e^{-i\phi})^{-1}]. \quad (3.11)$$

Since $|\xi_m|$ and $|\alpha|$ are less than 1 we may expand each term of (3.11) in a power series and obtain for $m\geq 1$

$$k_m = m^{-1} \sum_{l=1}^{\infty} (\xi_{2l-1}{}^m - \xi_{2l}{}^m), \quad (3.12a)$$

$$k_{-m} = -m^{-1}[\alpha^m + \sum_{l=1}^{\infty} (\xi_{2l}{}^m - \xi_{2l-1}{}^m)]. \quad (3.12b)$$

We may then combine (3.6) with (3.10) and (3.12) to obtain as $n\to\infty$

$$R_n \sim G^n P, \quad (3.13)$$

where

$$P = \prod_{m=1}^{\infty} [(1-\alpha\xi_{2m-1})(1-\alpha\xi_{2m})^{-1}]$$
$$\times \prod_{m=1}^{\infty}\prod_{m'=1}^{\infty} [(1-\xi_{2m}\xi_{2m'-1})^2(1-\xi_{2m}\xi_{2m'})^{-1} \times(1-\xi_{2m-1}\xi_{2m'-1})^{-1}]. \quad (3.14)$$

When T is large, it is trivial to use (2.12) to expand the infinite products and find

$$\rho_N{}^x \sim \{\beta[1-\tfrac{1}{3}(1+\alpha^2)\beta^2+O(\beta^4)]\}^N[1-\tfrac{2}{3}\alpha^2\beta^2+O(\beta^4)]. \quad (3.15)$$

This is valid for $0\leq\alpha\leq 1$ but is useful only when $\alpha\beta\ll 1$.

In the low-temperature case, this expansion breaks down. We now must asymptotically expand G and P by first rewriting them in terms of contour integrals. This procedure is somewhat different in the isotropic and anisotropic cases. We treat the anisotropic case here and return to the isotropic case in Sec. 6.

A. Expansion of G

To convert the logarithm of the infinite product (3.10) into a contour integral, we note that because the products in the numerator and denominator converge separately we may write

$$\ln G = \ln\beta + \sum_{m=1}^{\infty} (-1)^m \ln[(2\beta\pi^{-1})^2(2m)^{-2}\alpha\xi_m{}^{-1}]. \quad (3.16)$$

We then convert this series into a contour integral by using the fact that $\csc\pi m$ has poles with residue $(-1)^m/\pi$ at all integral values of m. Therefore,

$$\ln G = \ln\beta + (2i)^{-1}\int_C dm\, \csc\pi m\, \ln[(2\beta\pi^{-1})^2 m^{-2}\alpha\xi_m{}^{-1}], \quad (3.17)$$

where the contour C encircles all poles at positive values of m once in the counterclockwise direction. We now deform the contour of integration to the path $\mathrm{Re}\,m=\theta$ where $0<\theta<1$. The integrand has no singularities between these two paths and the contribution from the two arcs at infinity clearly vanishes. Therefore,

$$\ln G = \ln\beta - (2i)^{-1}\int_{-i\infty+\theta}^{i\infty+\theta} dm\, \csc\pi m \{\ln(2\beta\pi^{-1})^2 + \ln m^{-2} + \ln\tfrac{1}{2}[1+\alpha^2+(\tfrac{1}{2}\beta^{-1}\pi m)^2 + [((1-\alpha)^2+(\tfrac{1}{2}\beta^{-1}\pi m)^2)((1+\alpha)^2+(\tfrac{1}{2}\beta^{-1}\pi m)^2)]^{1/2}]\}. \quad (3.18)$$

The residue of the last term at $m=0$ is zero. Now

$$(2i)^{-1}\int_{-i\infty+\theta}^{i\infty+\theta} dm\, \csc\pi m\, \ln m = -\tfrac{1}{2}\ln(\pi/2), \quad (3.19)$$

so the first three terms of (3.18) cancel. Rewrite the remaining term by letting $m=iy$ and let $\theta\to 0$ (keeping y in the lower half-plane whenever there are singularities on the real y axis) to obtain

$$\ln G = -(2i)^{-1}\int_{-\infty}^{\infty} dy\, \mathrm{csch}\pi y\, \ln\tfrac{1}{2}\{1+\alpha^2-(\tfrac{1}{2}\beta^{-1}\pi y)^2 + [((1-\alpha)^2-(\tfrac{1}{2}\beta^{-1}\pi y)^2)[(1+\alpha)^2-(\tfrac{1}{2}\beta^{-1}\pi y)^2]]^{1/2}\}. \quad (3.20)$$

The square root is defined positive when $y=0$. Since the real part of the logarithm is a symmetric function of y, it gives no contribution and we readily find

$$\ln G = \ln\tanh[\beta(1+\alpha)] - \beta\pi^{-1}\int_{2(1-\alpha)}^{2(1+\alpha)} dt\, \mathrm{csch}\, t\beta \times\arctan\{[(\tfrac{1}{4}t^2-(1-\alpha)^2)((1+\alpha)^2-\tfrac{1}{4}t^2)]^{1/2} \times[1+\alpha^2-\tfrac{1}{4}t^2]^{-1}\}. \quad (3.21)$$

This reduction is exact. The second term of (3.21) is negative, so if we ignore it we obtain the upper bound on $\rho_N{}^x$ of

$$\rho_N{}^x \leq \mathrm{const}\times\tanh^N[\beta(1+\alpha)], \quad (3.22)$$

which was obtained by LSM.

In the low-temperature regime the first term of (3.21) is exponentially smaller than the second term and must be discarded. To obtain an asymptotic evaluation of the integral as $\beta\to\infty$ we note that if $\alpha<1$ we may replace $\operatorname{csch}\beta t$ by $2e^{-t\beta}$ and if $\alpha\neq0$ we may replace the upper limit by ∞. Make the change of variable

$$s^2=\tfrac{1}{2}t-(1-\alpha) \tag{3.23}$$

and expand

$$\arctan\{s[(2(1-\alpha)+s^2)(4\alpha-2(1-\alpha)s-s^4)]^{1/2}\times[2\alpha-2s^2(1-\alpha)-s^4]^{-1}\}=\sum_{m=0}^{\infty}A_m{}^G s^{2m+1}, \tag{3.24}$$

where the first few terms are

$$A_0{}^G=[2(\alpha^{-1}-1)]^{1/2},$$
$$A_1{}^G=\tfrac{1}{12}\sqrt{2}\alpha^{-3/2}(1-\alpha)^{-1/2}[3\alpha+(4-3\alpha)(1-\alpha)^2]. \tag{3.25}$$

Then if we integrate term by term we find the desired expansion

$$G\sim\exp\{-(2\pi\beta)^{-1/2}\exp[-2\beta(1-\alpha)]\times\sum_{m=0}^{\infty}3\cdot5\cdots(2m+1)(4\beta)^{-m}A_m{}^G\}. \tag{3.26}$$

B. Expansion of P

We convert P into a contour integral in a manner identical to the foregoing. The double products in P are converted into double integrals. The contributions to these integrals of the poles at $m=0$ and $m'=0$ are single integrals which cancel the single integral arising from the single product. Therefore, we obtain

$$P=(1-\alpha^2)^{1/4}\exp\left(\frac{1}{4}\int_{-i\infty+\theta}^{i\infty+\theta}dm\int_{-i\infty+\theta}^{i\infty+\theta}dm'\csc\pi m\csc\pi m'\times\ln[(1-\xi_m\xi_{m'})(1-\alpha^2)(1-\alpha\xi_m)^{-1}(1-\alpha\xi_{m'})^{-1}]\right). \tag{3.27}$$

Only the real part of the logarithm contributes to the integral and we find

$$P=(1-\alpha^2)^{1/4}\exp\left(\pi^{-2}\beta^2\int_{2(1-\alpha)}^{2(1+\alpha)}dt\times\int_{2(1-\alpha)}^{2(1+\alpha)}dt'\operatorname{csch}\beta t\operatorname{csch}\beta t'P(t,t')\right), \tag{3.28}$$

where

$$P(t,t')=\ln\left(\frac{1+\{B(t)B(t')[1-A(t)A(t')]^{-2}\}^{1/2}}{1-\{B(t)B(t')[1-A(t)A(t')]^{-2}\}^{1/2}}\right), \tag{3.29}$$

$$A(t)=\tfrac{1}{2}(\alpha^{-1}+\alpha-\tfrac{1}{4}\alpha^{-1}t^2), \tag{3.30a}$$

and

$$B(t)=\tfrac{1}{4}\alpha^{-2}[\tfrac{1}{4}t^2-(1-\alpha)^2][(1+\alpha)^2-\tfrac{1}{4}t^2]. \tag{3.30b}$$

We obtain a low-temperature expansion by using the substitution (3.23) and expanding

$$P(s,s')=\ln[(s+s')(s-s')^{-1}]^2+ss'\sum_{m=0}^{\infty}\sum_{m'=0}^{\infty}A_{m,m'}{}^P s^{2m}s^{2m'}. \tag{3.31}$$

We then find for $0<\alpha<1$

$$P\sim(1-\alpha^2)^{1/4}\exp\left(\pi^{-2}4^3\beta^2\exp[-4\beta(1-\alpha)]\int_0^\infty ds\int_0^\infty ds'\exp[-2\beta(s^2+s'^2)]\times ss'\{\ln[(s+s')(s-s')^{-1}]^2+ss'\sum_{m=0}^{\infty}\sum_{m'=0}^{\infty}A_{m,m'}{}^P s^{2m}s'^{2m}\}\right). \tag{3.32}$$

The first integral may be evaluated by transforming to polar coordinates as

$$\beta^2\int_0^\infty ds\int_0^\infty ds'\exp[-2\beta(s^2+s'^2)]ss'\ln[(s+s')(s-s')^{-1}]^2=\frac{1}{4}\int_0^{\pi/2}d\theta\cos\theta\sin\theta\ln|(\cos\theta+\sin\theta)/(\cos\theta-\sin\theta)|=\tfrac{1}{16}\pi. \tag{3.33}$$

Therefore, we obtain asymptotically at low temperatures

$$P\sim(1-\alpha^2)^{1/4}\exp\{\exp[-4\beta(1-\alpha)]\pi^{-1}[4+(2\beta)^{-1}\sum_{m=0}^{\infty}\sum_{m'=0}^{\infty}A_{m,m'}{}^P(4\beta)^{-m-m'}3\cdot5\cdots(2m+1)\times3\cdot5\cdots(2m'+1)]\}. \tag{3.34}$$

C. Asymptotic Behavior of $\rho_N{}^x$

We now may combine the expansions of the preceding two subsections to obtain the explicit asymptotic behavior of $\rho_N{}^x$ as $N\to\infty$, $0<\alpha<1$, and T is small:

$$\rho_N{}^x\sim(1-\alpha^2)^{1/2}\exp\{-N[(2\pi\beta)^{-1/2}\exp(-2\beta(1-\alpha))\sum_{m=0}^{\infty}3\cdot5\cdots(2m+1)(4\beta)^{-m}A_m{}^G]\}\times\exp\{\pi^{-1}\exp[-4\beta(1-\alpha)][8+\beta^{-1}\sum_{m=0}^{\infty}\sum_{m'=0}^{\infty}A_{m,m'}{}^P(4\beta)^{-m-m'}3\cdot5\cdots(2m+1)3\cdot5\cdots(2m'+1)]\}. \tag{3.35}$$

In this asymptotic expansion N and β are *independently* large. We may therefore keep N large enough so that this asymptotic expansion is valid and take the $T\to 0$ limit to find that in the ground state[5]

$$\lim_{N\to\infty} \rho_N{}^x=(1-\alpha^2)^{1/2}. \tag{3.36}$$

4. CORRELATION $\rho_N{}^y$ FOR $\alpha<1$

When $0<\alpha<1$ the asymptotic expansion of $\rho_N{}^y$ is more complicated than the expansion of $\rho_N{}^x$ carried out in the previous section. We need to evaluate $R_n(\alpha^{-1})$ for $\alpha<1$, and it is not possible to do this merely by use of Szego's theorem. This difficulty is the same one encountered by Wu[3] in his analysis of the Toeplitz determinants which arise in the correlation of two spins on the same row of the two-dimensional Ising model. Wu's very clear analysis is developed in sufficient generality that we need not repeat it here but will simply quote the needed results and refer the reader to his paper for proofs.

The evaluation of $R_n(\alpha^{-1})$ for $\alpha<1$ parallels Wu's evaluation of S_N for $T>T_c$ (Sec. 2w). We first define

$$c_j=a_{j-1}=-(2\pi)^{-1}\int_0^{2\pi} d\phi\, e^{-ij\phi}[(1-\alpha e^{i\phi})/(1-\alpha e^{-i\phi})]^{1/2} \times \tanh\{\beta[(1-\alpha^{-1}e^{i\phi})(1-\alpha^{-1}e^{-i\phi})]^{1/2}\}, \tag{4.1}$$

where the square roots are positive at $e^{i\phi}=-1$. Call the $n\times n$ determinant formed from the c's

$$\bar{R}_n(\alpha^{-1})=\begin{vmatrix} c_0 & \cdots & c_{-n+1} \\ \cdot & \cdots & \cdot \\ \cdot & \cdots & \cdot \\ \cdot & \cdots & \cdot \\ c_{n-1} & \cdots & c_0 \end{vmatrix}. \tag{4.2}$$

We extract a (-1) from each element of (4.2) and apply Szego's theorem to $(-1)^n\bar{R}_n$. The only difference from the expansion of R_n of the last section is that β is replaced by $\beta\alpha^{-1}$, so if we explicitly indicate the dependence on β,

$$\lim_{n\to\infty}(-1)^n\bar{R}_n(\alpha,\beta)=\lim_{n\to\infty}R_n(\alpha,\beta\alpha^{-1}). \tag{4.3}$$

We define x_m by

$$\sum_{m=0}^{n} c_{l-m}x_m=\delta_{l0}, \tag{4.4}$$

so that

$$R_n=(-1)^n\bar{R}_{n+1}x_n. \tag{4.5}$$

Wu shows that if

$$C(\xi)=\sum_{l=-\infty}^{\infty} c_l\xi^l \tag{4.6}$$

is such that $\ln C(\xi)$ is continuous and periodic on the unit circle, and if we may write for $|\xi|=1$

$$[C(\xi)]^{-1}=P(\xi)Q(\xi^{-1}) \tag{4.7}$$

such that $P(\xi)$ and $Q(\xi)$ are both analytic for $|\xi|<1$ and continuous and nonzero for $|\xi|\leq 1$, then

$$x_n \doteqdot (2\pi i)^{-1}\oint d\xi\, \xi^{n-1}P(\xi^{-1})Q(\xi)^{-1}, \tag{4.8}$$

where the integration is around the unit circle. Here the symbol $\doteqdot$ means that if we fix $\alpha<1$ both sides of the equation have the same asymptotic expansion as $n\to\infty$. For our case $C(\xi)$ is given by

$$C(\xi)=-\bar{G}(1-\alpha e^{i\phi})\prod_{m=1}^{\infty}(1-\xi\bar{\xi}_{2m})(1-\xi\bar{\xi}_{2m-1})^{-1} \times(1-\xi^{-1}\bar{\xi}_{2m})(1-\xi^{-1}\bar{\xi}_{2m-1})^{-1}. \tag{4.9}$$

Here $\bar{\xi}_m$ and $\bar{G}$ are obtained from ξ of (2.9) and G of (3.10) by the replacement $\beta\to\beta\alpha^{-1}$. We may therefore choose

$$P(\xi)=-\bar{G}^{-1}(1-\alpha\xi)^{-1}\prod_{m=1}^{\infty}(1-\xi\bar{\xi}_{2m-1})(1-\xi\bar{\xi}_{2m})^{-1} \tag{4.10}$$

and

$$Q(\xi)=\prod_{m=1}^{\infty}(1-\xi\bar{\xi}_{2m-1})(1-\xi\bar{\xi}_{2m})^{-1} \tag{4.11}$$

to obtain

$$x_n\doteqdot -(2\pi i)^{-1}\bar{G}^{-1}\oint d\xi\,\xi^{n-1}(1-\alpha\xi^{-1})^{-1} \times\prod_{m=1}^{\infty}[(1-\xi^{-1}\bar{\xi}_{2m-1})(1-\xi^{-1}\bar{\xi}_{2m})^{-1} \times(1-\xi\bar{\xi}_{2m})(1-\xi\bar{\xi}_{2m-1})^{-1}]. \tag{4.12}$$

This may be rewritten, using the infinite-product representation of the hyperbolic tangent (3.9), as

$$x_n\doteqdot -(2\pi i)^{-1}\oint d\xi\,\xi^{n-1}\left(\frac{1-\alpha\xi}{1-\alpha\xi^{-1}}\right)^{1/2}\coth\{\beta\alpha^{-1}[(1-\alpha\xi)(1-\alpha\xi^{-1})]^{1/2}\}\prod_{m=1}^{\infty}[(1-\xi\bar{\xi}_{2m})(1-\xi\bar{\xi}_{2m-1})^{-1}]^2. \tag{4.13}$$

The remaining product in (4.13) may be rewritten as

$$\prod_{m=1}^{\infty}[(1-\xi\bar{\xi}_{2m})/(1-\xi\bar{\xi}_{2m-1})]^2=(1-\alpha\xi)^{-1}\exp\left(-2\beta\pi^{-1}\int_{2(\alpha^{-1}-1)}^{2(\alpha^{-1}+1)}dt\,\operatorname{csch}\beta t\,\operatorname{Im}\ln[(1-\xi\bar{\xi}(t))(1-\alpha\xi)^{-1}]\right), \tag{4.14}$$

where

$$\bar{\xi}(t)=\tfrac{1}{2}\alpha\{1+\alpha^{-2}-\tfrac{1}{4}t^2-[((\alpha^{-1}-1)^2-\tfrac{1}{4}t^2)((\alpha^{-1}+1)^2-\tfrac{1}{4}t^2)]\}^{1/2}. \tag{4.15}$$

[5] This limit is closely related to the end-to-end correlation function in a chain with free boundary conditions given in (2.79) of LSM.

Therefore, (4.13) may be expressed as

$$x_n \doteq -(2\pi i)^{-1}\oint d\xi\, \xi^{n-1}[(1-\alpha\xi)(1-\alpha\xi^{-1})]^{-1/2}\coth\Big[\beta\alpha^{-1}[(1-\alpha\xi)(1-\alpha\xi^{-1})]^{1/2} \times \exp\Big(-2\beta\pi^{-1}\int_{2(\alpha^{-1}-1)}^{2(\alpha^{-1}+1)} dt\, \mathrm{csch}\beta t\, \mathrm{Im}\ln[(1-\xi\bar{\xi}(t))(1-\alpha\xi)^{-1}]\Big)\Big]. \quad (4.16)$$

It remains to obtain an asymptotic expansion of (4.16) for large n. To do this, we use the partial-fraction decomposition of the hyperbolic cotangent and note that the only singularities of the integrand inside the unit circle are simple poles at $\xi=\xi_{2m}$ and α to write

$$x_n \doteq -\beta^{-1}\alpha^n(\alpha^{-1}-\alpha)^{-1}\exp\Big(-2\beta\pi^{-1}\int_{2(\alpha^{-1}-1)}^{2(\alpha^{-1}+1)} dt\,\mathrm{csch}\beta t\,\mathrm{Im}\ln[(1-\alpha\bar{\xi}(t))(1-\alpha^2)^{-1}]\Big) - \beta^{-1}2\sum_{k=1}^{\infty}\bar{\xi}_{2k}{}^n(\bar{\xi}_{2k}{}^{-1}-\bar{\xi}_{2k})^{-1} \times \exp\Big(-2\beta\pi^{-1}\int_{2(\alpha^{-1}-1)}^{2(\alpha^{-1}+1)} dt\,\mathrm{csch}\beta t\,\mathrm{Im}\ln[(1-\xi_{2k}\bar{\xi}(t))(1-\xi_{2k}\alpha)^{-1}]\Big). \quad (4.17)$$

When $T>0$ is fixed and $n\to\infty$ the second term in (4.17) is exponentially smaller than the first and does not contribute to an asymptotic expansion. We then obtain

$$\rho_N{}^y \sim \bar{G}^{N+2}\alpha^{N+2}\beta^{-2}\{\prod_{m=1}^{\infty}[(1-\alpha\bar{\xi}_{2m})/(1-\alpha\bar{\xi}_{2m-1})]\prod_{m=1}^{\infty}\prod_{m'=1}^{\infty}[(1-\bar{\xi}_{2m}\bar{\xi}_{2m'-1})(1-\bar{\xi}_{2m}\bar{\xi}_{2m'})^{-1}(1-\bar{\xi}_{2m-1}\bar{\xi}_{2m'-1})^{-1}]\}^2. \quad (4.18)$$

When T is large, we expand (4.18) as

$$\rho_N{}^y \sim \{\beta[1-(\alpha^{-2}+1)\tfrac{1}{3}\beta^2+O(\beta^4)]\}^N[1-\tfrac{2}{3}\alpha^{-2}\beta^2+O(\beta^4)]. \quad (4.19)$$

This is identical to the corresponding high-temperature expansion of $\rho_N{}^x$ [Eq. (3.15)] with the replacement $\alpha\leftrightarrow\alpha^{-1}$.

When T is small, we asymptotically expand (4.14) as

$$\prod_{m=1}^{\infty}(1-\alpha\bar{\xi}_{2m})/(1-\alpha\bar{\xi}_{2m-1}) = (1-\alpha^2)^{-1/2}\exp\{-(2\pi\beta\alpha^{-1})^{-1/2}\exp[-2\beta(\alpha^{-1}-1)]\sum_{m=0}^{\infty}3\cdot5\cdots(2m+1)(4\alpha^{-1}\beta)^{-m}A_m{}^{(1)}\}, \quad (4.20)$$

where $A_m{}^{(1)}$ are defined by

$$\sum_{m=0}^{\infty}A_m{}^{(1)}s^{2m+1} = \arctan\{s[(2(1-\alpha)+s^2)(4\alpha-2(1-\alpha)s^2-s^4)]^{1/2}[2(1-\alpha)+2s(1-\alpha)s^2+s^4]^{-1}\}. \quad (4.21)$$

The first two $A_m{}^{(1)}$ are

$$A_0{}^{(1)} = [2\alpha/(1-\alpha)]^{1/2}, \quad (4.22a)$$

$$A_1{}^{(1)} = -\tfrac{1}{12}\sqrt{2}\alpha^{-1/2}(1-\alpha)^{-3/2}(3+2\alpha-9\alpha^2). \quad (4.22b)$$

Thus for T small

$$\rho_N{}^y \sim \alpha^{N+2}\beta^{-2}(1-\alpha)^{-3/2}\exp\{-(N+2)[(2\pi\alpha^{-1}\beta)^{1/2}e^{-2\beta(\alpha^{-1}-1)}\sum_{m=0}^{\infty}3\cdot5\cdots(2m+1)(4\alpha^{-1}\beta)^mA_m{}^G]\} \times \exp\{-[(2\alpha/\pi\beta)^{1/2}\exp(-2\beta(\alpha^{-1}-1))\sum_{m=0}^{\infty}3\cdot5\cdots(2m+1)(4\alpha^{-1}\beta)^{-m}A_m{}^{(1)}]\}. \quad (4.23)$$

This is to be compared with (2.15) and (3.35).

In order for this last expansion to be useful, we must have $\beta(1-\alpha)\gg1$. However, if for large but fixed n, β becomes too large, the approximation of neglecting the infinite series in (4.17) no longer gives the correct asymptotic behavior. We study this regime where n and β are comparable as we did in Sec. 2 by defining

$$q_y = \tfrac{1}{4}n\beta^{-2}(\alpha^{-2}-1)^{-1} = \tfrac{1}{4}[\tfrac{1}{2}(N+1)]\beta^{-2}(\alpha^{-2}-1)^{-1}, \quad (4.24)$$

where [ ] means the greatest integer contained in the brackets, and letting n and $\beta\to\infty$ with q_y held fixed. In this limit, all the integrals in the expression for

$$\lim_{n\to\infty}(-1)^nR_n$$

and in (4.17) are exponentially small and do not contribute to the asymptotic expansion. The expression for $R_n(\alpha^{-1})$ then simplifies to

$$R_n(\alpha^{-1}) \sim (1-\alpha^2)^{1/4}\beta^{-1}\{\alpha^n(\alpha^{-1}-\alpha)^{-1} + 2\sum_{k=1}^{\infty}\bar{\xi}_{2k}{}^n(\bar{\xi}_{2k}{}^{-1}-\bar{\xi}_{2k})^{-1}\}. \quad (4.25)$$

We follow the procedure of Sec. 2 and obtain

$$R_n(\alpha^{-1})\sim(1-\alpha^2)^{-1/4}(q_y/\pi n)^{1/2}\alpha^n \times\left[1+n^{-1}(1+\alpha^2)(1-\alpha^2)^{-1}\left(q_y\frac{\partial}{\partial q_y}+\tfrac{1}{2}q_y^2\frac{\partial^2}{\partial q_y^2}\right)\right] \times[q_y^{-1/2}+2q_y^{-1/2}\sum_{m=1}^{\infty}e^{-m^2/4q_y}]. \quad (4.26)$$

From this we use (3.2) to obtain the desired answer:

$$\rho_N^y\sim2(1-\alpha^2)^{-1/2}\pi^{-1}N^{-1}\alpha^N\{[1+2\sum_{m=1}^{\infty}\exp(-m^2/4q_y)]^2 -\tfrac{1}{2}N^{-1}(1+\alpha^2)(1-\alpha^2)^{-1}[1+2\sum_{m=1}^{\infty}\exp(-m^2/4q_y)] \times[1+2\sum_{m=1}^{\infty}\exp(-m^2/4q_y)(1+2(m^2/2q_y)-(m^2/2q_y)^2)] +O(N^{-2})\}. \quad (4.27)$$

It should be noted that while the two terms explicitly shown here have the same dependence on N regardless of whether N is odd or even the $O(N^{-2})$ term *will* depend on the evenness or oddness of N. Finally, we may let $q_y\to0$ and we obtain the $T=0$ correlation

$$\rho_N^y\sim2(1-\alpha^2)^{-1/2}\pi^{-1}N^{-1}\alpha^N \times[1-\tfrac{1}{2}N^{-1}(1+\alpha^2)(1-\alpha^2)^{-1}+O(N^{-2})]. \quad (4.28)$$

5. CORRELATION ρ_N^x NEAR $T=0$

In Sec. 3 we were able to recover the $N\to\infty$ limit of ρ_N^x at $T=0$ from the nonzero-temperature result but were unable to recover the approach of ρ_N^x to this limit. We may recover this second term in ρ_N^x at $T=0$ from the nonzero-temperature case by using the methods of Sec. 3 of Wu's paper to evaluate the second term in the expansion of ρ_N^x when N and $\beta\to\infty$ and

$$q_x=\tfrac{1}{4}n\beta^{-2}(1-\alpha^2)^{-1} =\tfrac{1}{4}[\tfrac{1}{2}(N+1)]\beta^{-2}(1-\alpha^2)^{-1}=\alpha^{-2}q_y \quad (5.1)$$

is held fixed.

To compute the first correction to Szego's theorem, it is convenient to write R_n as

$$R_n(\alpha)=G^n\begin{vmatrix}\bar{a}_0 & \bar{a}_{-1} & \cdots & \bar{a}_{-n+1}\\ \bar{a}_1 & \bar{a}_0 & \cdots & \bar{a}_{-n+2}\\ \cdot & \cdot & \cdots & \cdot\\ \cdot & \cdot & \cdots & \cdot\\ \cdot & \cdot & \cdots & \cdot\\ \bar{a}_{n-1} & \bar{a}_{n-2} & \cdots & \bar{a}_0\end{vmatrix}, \quad (5.2)$$

where G is given by (3.10) and

$$\bar{a}_n=G^{-1}a_n=(2\pi)^{-1}\int_0^{2\pi}d\phi\, e^{-in\phi}(1-\alpha e^{-i\phi})\prod_{m=1}^{\infty}[(e^{i\phi}-\xi_{2m}) \times(e^{-i\phi}-\xi_{2m})(e^{i\phi}-\xi_{2m-1})^{-1}(e^{-i\phi}-\xi_{2m-1})^{-1}]. \quad (5.3)$$

We already know from (3.36) that if $N\to\infty$ and $\beta\to\infty$ in any fashion, then $R_n(\alpha)\to(1-\alpha^2)^{1/4}$, so we find from Wu's Eq. (3.4w) that

$$R_n(\alpha)\doteqdot(1-\alpha^2)^{1/4}\prod_{m=n}^{\infty}x_0(m), \quad (5.4)$$

where $x_0(m)$ is the zeroth component of the $m+1$ component vector defined by

$$\sum_{j=0}^{m}\bar{a}_{k-j}x_j=\delta_{k0}. \quad (5.5)$$

Wu shows that (3.13w)

$$x_0(m)\doteqdot1-(2\pi i)^{-2}\oint d\xi\,\xi^mQ(\xi^{-1})P(\xi)^{-1} \times\oint d\xi'\,P(\xi')Q(\xi'^{-1})^{-1}\xi'^{-m-1}(\xi'-\xi)^{-1}, \quad (5.6)$$

where the path of the ξ' integration is indented outward at $\xi'=\xi$ and

$$\sum_{m=-\infty}^{\infty}\bar{a}_m\xi^m=P(\xi)^{-1}Q(\xi^{-1})^{-1} \quad (5.7)$$

for $|\xi|=1$. The functions $P(\xi)$ and $Q(\xi)$ have the same analyticity properties required in Sec. 4 and for this application are specifically given as

$$Q(\xi)=(1-\alpha\xi)^{-1}\prod_{m=1}^{\infty}[(1-\xi\xi_{2m-1})(1-\xi\xi_{2m})^{-1}] \quad (5.8)$$

and

$$P(\xi)=\prod_{m=1}^{\infty}[(1-\xi\xi_{2m-1})(1-\xi\xi_{2m})^{-1}]. \quad (5.9)$$

We use (5.6), (5.8), and (5.9) in (5.4) and expand the infinite product to obtain asymptotically

$$R_n\doteqdot(1-\alpha^2)^{1/4}\{1+\sum_{m=n}^{\infty}[x_0(m)-1]\}\doteqdot(1-\alpha^2)^{1/4}\Big(1+(2\pi)^{-2}\oint d\xi\,\xi^n(1-\alpha\xi^{-1})^{-1} \times\prod_{m=1}^{\infty}[(1-\xi^{-1}\xi_{2m-1})(1-\xi^{-1}\xi_{2m})^{-1}(1-\xi\xi_{2m})(1-\xi\xi_{2m-1})^{-1}]\oint d\xi'\,(\xi'-\xi)^{-2}\xi'^{-n}(1-\alpha\xi'^{-1}) \times\prod_{m=1}^{\infty}[(1-\xi'\xi_{2m-1})(1-\xi'\xi_{2m})^{-1}(1-\xi'^{-1}\xi_{2m})(1-\xi'^{-1}\xi_{2m-1})^{-1}]\Big). \quad (5.10)$$

We may use the infinite-product representation of coth and (4.14) to rewrite this as

$$R_n \doteq (1-\alpha^2)^{1/4}\Big\{1+(2\pi)^{-2}G^2 \oint d\xi\, \xi^n[(1-\alpha\xi)(1-\alpha\xi^{-1})]^{-1/2} \coth\{\beta[(1-\alpha\xi)(1-\alpha\xi^{-1})]^{1/2}\}$$

$$\times \exp\Big\{-2\beta\pi^{-1}\int_{2(1-\alpha)}^{2(1+\alpha)} dt\, \mathrm{csch}t\, \mathrm{Im}\ln[(1-\xi\xi(t))(1-\alpha\xi)^{-1}]\Big\} \oint \xi'^{-n}(\xi'-\xi)^{-2}[(1-\alpha\xi')(1-\alpha\xi'^{-1})]^{1/2}$$

$$\times \coth\{\beta[(1-\alpha\xi')(1-\alpha\xi'^{-1})]^{1/2}\} \exp\Big\{-2\beta\pi^{-1}\int_{2(1-\alpha)}^{2(1+\alpha)} dt\, \mathrm{csch}\beta t\, \mathrm{Im}\ln[(1-\xi'^{-1}\xi(t))(1-\alpha\xi'^{-1})^{-1}]\Big\}\Big\}. \quad (5.11)$$

In the N, $\beta\to\infty$ limit, the integrals and the factor G^2 in (5.11) are asymptotically equal to 1. We then use the partial-fraction decomposition of coth to find

$$R_n \doteq (1-\alpha^2)^{1/4}[1+2\beta^{-2}\alpha^{-2}\sum_{m=-\infty}^{\infty} \xi_{2m}^{n+1}(\xi_{2m}^{-1}-\xi_{2m})^{-1}$$

$$\times \sum_{m'=1}^{\infty} \xi_{2m'}^{n-1}(\xi_{2m'}^{-1}-\xi_{2m})^{-2}(\xi_{2m'}-\xi_{2m'}^{-1})^{-1}(1-\alpha\xi_{2m'})(1-\alpha\xi_{2m'}^{-1})]. \quad (5.12)$$

We now expand this expression for fixed q_x using the methods of Secs. 2 and 4 and use the result in (3.2) to obtain the desired answers:

$$\rho_{2n}^x \sim (1-\alpha^2)^{1/2}\{1+4(2n)^{-2}\alpha^{2n}(\alpha^{-1}-\alpha)^{-2}\pi^{-1}[F_1-(1+\alpha^2)(1-\alpha^2)^{-1}(2n)^{-1}F_2+O((2n)^{-2})]\} \quad (5.13a)$$

and

$$\rho_{2n-1}^x \sim (1-\alpha^2)^{1/2}\{1+2(2n-1)^{-2}\alpha^{2n-1}(\alpha^{-1}-\alpha)^{-2}\pi^{-1}$$

$$\times[(\alpha+\alpha^{-1})F_1+(2n-1)^{-1}[2(\alpha^{-1}-\alpha)F_1-(\alpha+\alpha^{-1})^2(\alpha^{-1}-\alpha)^{-1}F_2]+O((2n-1)^2)]\}, \quad (5.13b)$$

where

$$F_1=[1+2\sum_{m=1}^{\infty}\exp(-m^2/4q_x)][1+2\sum_{m=1}^{\infty}\exp(-m^2/4q_x)(1-m^2/2q_x)] \quad (5.14a)$$

and

$$F_2=\tfrac{1}{2}[1+2\sum_{m=1}^{\infty}\exp(-m^2/4q_x)]\{\tfrac{9}{2}+\sum_{m=1}^{\infty}\exp(-m^2/4q_x)[9-3(m^2/2q_x)-7(m^2/2q_x)^2+(m^2/2q_x)^3]\}$$

$$-\tfrac{1}{2}[1+2\sum_{m=1}^{\infty}\exp(-m^2/4q_x)(1-m^2/2q_x)]\{-\tfrac{5}{2}+\sum_{m=1}^{\infty}\exp(-m^2/4q_x)[-5+2(m^2/2q_x)+(m^2/2q_x)^2]\}. \quad (5.14b)$$

These results should be contrasted with the comparable results for ρ_N^y given by (4.2) and for ρ_N^z given by (2.25) when $\alpha<1$, and by (2.29) when $\alpha=1$.

We finally are able to obtain asymptotic behavior of the ground-state correlation function by setting $q_x=0$. We find

$$\rho_{2n}^x \sim (1-\alpha^2)^{1/2}\{1+4(2n)^{-1}\alpha^{2n}(\alpha^{-1}-\alpha)^{-2}\pi^{-1}[1-\tfrac{7}{2}(1+\alpha^2)(1-\alpha^2)^{-1}(2n)^{-1}+O((2n)^{-2})]\} \quad (5.15a)$$

and

$$\rho_{2n-1}^x \sim (1-\alpha^2)^{1/2}\{1+2(2n-1)^{-2}\alpha^{2n-1}(\alpha^{-1}-\alpha)^{-2}\pi^{-1}$$

$$\times[\alpha+\alpha^{-1}+(2n-1)^{-1}[2(\alpha^{-1}-\alpha)-\tfrac{7}{2}(\alpha+\alpha^{-1})^2(\alpha^{-1}-\alpha)^{-1}]+O((2n-1)^{-2})]\}. \quad (5.15b)$$

6. CORRELATIONS ρ_N^x AND ρ_N^z FOR $\alpha=1$

The foregoing low-temperature asymptotic expansions of ρ_N^x and ρ_N^y have been restricted to the anisotropic case. We now wish to study the corresponding asymptotic behavior in the isotropic case when T is fixed and $N\to\infty$. When $T>0$ this may be done by applying Szego's theorem as we did in Sec. 3. In particular, we obtain a valid expression for $R_n(1)$ if we let $\alpha\to1$ in (3.13). Furthermore, expression (3.21) for

G is still valid if we let $\alpha \to 1$. However, the expression for P in terms of an integral given in Sec. 3 is not particularly suitable for taking the $\alpha \to 1$ limit. Instead, we choose to set $\alpha = 1$ at the outset and obtain

$$P = \beta^{-1/4} \exp\left\{ (2\beta/\pi)^2 \int_{-\infty}^{\infty} dt\, \mathrm{csch} 4\beta t \int_{-\infty}^{\infty} dt'\, \mathrm{csch} 4\beta t' \times \ln \left| [t(1-t'^2)^{1/2} + t'(1-t^2)^{1/2}](t+t')^{-1} \right| \right\}, \quad (6.1)$$

where the square roots are defined positive at t and $t' = 0$ and the contours of integration are in the lower half-planes. When T is small, we expand the integrand of (6.1) about $t, t' = 0$ as

$$\ln \left| [t(1-t'^2)^{1/2} + t'(1-t^2)^{1/2}](t+t')^{-1} \right| = -\tfrac{1}{2} \sum_{m=1}^{\infty} \sum_{m=1}^{\infty} I_{m,m'}{}^P t^{2m-1} t'^{2m'-1}, \quad (6.2)$$

where

$$I_{0,0}{}^P = 1 \quad \text{and} \quad I_{1,0}{}^P = I_{0,1}{}^P = \tfrac{1}{4}. \quad (6.3)$$

Then, if we integrate term by term we obtain the asymptotic expansion

$$P \sim \beta^{-1/4} \exp\{ -\sum_{m=1}^{\infty} \sum_{m'=1}^{\infty} (-1)^{m+m'} (\pi/4\beta)^{2(m+m'-1)} \times (8mm')^{-1} (2^{2m}-1)(2^{2m'}-1) B_{2m} B_{2m'} I_{m,m'}{}^P \}, \quad (6.4)$$

where we have used an integral representation of Bernoulli's numbers[6] B_{2m}.

We obtain a useful low-temperature expansion for $G(1)$ by first defining $I_m{}^G$ by

$$\arctan\{ 2x[1-x^2]^{1/2} [1-2x^2]^{-1} \} = \sum_{m=1}^{\infty} x^{2m-1} I_m{}^G, \quad (6.5)$$

where the first two $I_m{}^G$ are given by

$$I_1{}^G = 2,\ I_2{}^G = \tfrac{1}{3}. \quad (6.6)$$

Using this in (3.21) we find

$$G(1) \sim \exp\{ -\sum_{m=1}^{\infty} (\pi/4\beta)^{2m-1} (-1)^{m+1} (2m)^{-1} \times (2^{2m}-1) B_{2m} I_m{}^G \}. \quad (6.7)$$

[6] Reference 4, Vol. 1, p. 39.

We therefore obtain, when $N \to \infty$ with T small and fixed,

$$\rho_N{}^x(1) = \rho_N{}^y(1) \sim \beta^{-1/2} \exp\{ -N[\sum_{m=1}^{\infty} (-1)^{m+1} \times (\pi/4\beta)^{2m-1} (2m)^{-1} (2^{2m}-1) B_{2m} I_m{}^G] \} \times \exp\{ -\sum_{m=1}^{\infty} \sum_{m'=1}^{\infty} (-1)^{m+m'} (\pi/4\beta)^{2(m+m'-1)} (4mm')^{-1} \times (2^{2m}-1)(2^{2m'}-1) B_{2m} B_{2m'} I_{m,m'}{}^P \}. \quad (6.8)$$

This isotropic low-temperature asymptotic expansion is to be contrasted with the corresponding anisotropic expansion [Eqs. (3.35) and (4.23)].

We finally obtain the ground-state correlation functions by noting that at $T = 0$ the determinant $R_n(1)$ is the determinant exactly evaluated in Sec. 4 of Wu. Using the asymptotic expansion given there we find as $N \to \infty$

$$\rho_N{}^x(1) = \rho_N{}^y(1) \sim 4 e^{1/2} 2^{2/3} A^{-6} N^{-1/2} \times [1 - (-1)^N \tfrac{1}{8} N^{-2} + \cdots], \quad (6.9)$$

where $A = 1.2824\cdots$ is Glaisher's constant. This is to be compared with the previous result of LSM which said that $\rho_N{}^x(1)$ was bounded by a constant times $N^{-0.4053}$.

In marked contrast to all other correlation functions of the X-Y model, this correlation approaches its $N \to \infty$ limit in a nonintegrable fashion. It has recently been shown by several authors[7] that if at some temperature

$$\rho_N{}^i \underset{N\to\infty}{\longrightarrow} N^{-(d-2+\eta)},$$

where d is the dimensionality of the system and $\eta \leq 2$ then, at that temperature, when $H_i \to 0$ the magnetization M_i of the system is given by

$$\mathrm{sgn}(H_i) K \,|\, H_i \,|^{1/\delta}, \quad (6.10)$$

where K is some constant and

$$\delta = -1 + 2d/(d-2+\eta). \quad (6.11)$$

Therefore, in the X-Y model at $T = 0$ as $H \to 0$

$$M_x \to \mathrm{sgn}(H_x) K \,|\, H_x \,|^{1/3}. \quad (6.12)$$

[7] M. E. Fisher, J. Appl. Phys. **38**, 981 (1967); J. D. Gunton and M. J. Buckingham, Phys. Rev. Letters **20**, 143 (1968); B. M. McCoy and T. T. Wu (to be published).