in terms of a moment of the phase-space density. For example, if the total turbulent energy input $\epsilon = \langle H\rangle/\Omega - P_0/(\gamma-1)$ is known, then $\beta=\beta(\epsilon)$ is implicitly given by the integral relation

$$\int\cdots\int\left(\frac{H}{\Omega}-\frac{P_0}{\gamma-1}\right) f(\beta H)\prod_{\{\vec{k}\}}(d^6\vec{p}_{\vec{k}}\, d^6\vec{q}_{\vec{k}})=\epsilon \ . \tag{63}$$

In the formal derivation of Eq. (62), it has been assumed that the plasma is in contact with an appropriate "large" system, which sustains the fully developed stationary turbulence. Equation (62) may, therefore, be designated as the canonical distribution of the wave modes.

The phase-space density permits evaluation of the statistical behavior of the plasma as the average behavior of the ensemble of similar plasmas. The above considerations thus extend statistical mechanics to continuous, macroscopic electron plasmas.

V. CONCLUSION

The Hamiltonian dynamics and statistical mechanics of wave modes represent a theoretical basis for the analysis of nonlinear phenomena in electron plasmas, in particular violent fluctuations and stationary turbulence. Dissipation by collisional and collisionless interactions could not be included in the considerations because of the difficulties associated with the establishment of a variational principle for a continuous medium with dissipation. This idealized description is reflected in the constancy of the entropy of the wave modes with time, which expresses the reversibility of the basic field equations on which the canonical formalism rests:

$$\frac{dS}{dt}=-\kappa\int\cdots\int(1+\ln f)\left(\frac{\partial}{\partial t}+\vec{v}_{\{\vec{k}\}}\cdot\nabla_{\{\vec{k}\}}\right)f \times\prod_{\{\vec{k}\}}(d^6\vec{p}_{\vec{k}}\, d^6\vec{q}_{\vec{k}})=0 \ .$$

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$$\frac{\delta F[\Psi(x)]}{\delta\Psi(x)}=\lim_{\epsilon\to 0}\left(\frac{F[\Psi(x')+\epsilon\delta(x-x')]-F[\Psi(x')]}{\epsilon}\right).$$

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Off-Diagonal Time-Dependent Spin Correlation Functions of the X-Y Model*

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We consider the anisotropic one-dimensional X-Y model of Lieb, Schultz, and Mattis and study the three zero-temperature correlation functions $\rho_{\mu\nu}(R,t)=\langle S_1^\mu(0)\,S_{R+1}^\nu(t)\rangle$, where $\mu\nu=x,y,z$ but $\mu\neq\nu$. We obtain the first-order term of ρ_{xy} for $R\to\infty$ or $t\to\infty$ and exact expressions for ρ_{xz} and ρ_{yz}.

I. INTRODUCTION

We are interested in the one-dimensional X-Y model with an even number N of spin-$\frac{1}{2}$ particles and with an external magnetic field h in the z direction.[1,2] The Hamiltonian is

$$H=-\tfrac{1}{2}\sum_{i=1}^{N}(a_i^\dagger a_{i+1}+a_{i+1}^\dagger a_i+\gamma a_i^\dagger a_{i+1}^\dagger+\gamma a_{i+1}a_i) -h\sum_{i=1}^{N}(a_i^\dagger a_i-\tfrac{1}{2}) \ , \tag{1.1}$$

where $a_i^\dagger$ and a_i are the spin-$\frac{1}{2}$ raising and lowering operators, respectively, at site i. We choose periodic boundary conditions so that $a_{N+1}^\dagger=a_1^\dagger$ and $a_{N+1}=a_1$ and take $h\geq 0$ and $0<\gamma\leq 1$. Correlation functions are in general defined as

$$\rho_{\mu\nu}(R,t)=\langle S_1^\mu(0)S_{R+1}^\nu(t)\rangle\ , \qquad (1.2)$$

where $\mu, \nu = x, y, z$. $S_l^\mu(t)=\frac{1}{2}\sigma_l^\mu(t)$, where the $\sigma_l^\mu(t)$ are the Pauli matrices in the Heisenberg picture. R is the separation of the two spins, t is time, and $\langle\cdots\rangle$ indicates that the operators are averaged over the canonical ensemble.

The diagonal ($\mu=\nu$) correlation functions are well defined by (1.2) and have been previously studied.[3-6] However, the off-diagonal ones ($\mu\neq\nu$) are not uniquely defined by (1.2). If one has a magnetic field h_x on the system in the x direction, one finds that the two limits in

$$\lim_{h_x\to 0^\pm}\ \lim_{N\to\infty}\ \rho_{\mu\nu}(R,t) \qquad (1.3)$$

cannot be arbitrarily interchanged. If one takes the limits as given in (1.3), one can show that $\rho_{xz}(R,t)$ at zero temperature and $h<1$ is nonzero. If one reverses the limits, $\rho_{xz}(R,t)=\rho_{yz}(R,t)=0$ for all temperature and $0\le h$. The method we use defines the off-diagonal $\rho_{\mu\nu}(R,t)$ by (1.2) and a limiting process of the form (1.3) with $h_x\to 0^\pm$.

Because of the limitations of our formalism we can only compute the zero-temperature correlation functions and, unless otherwise stated, we deal only with these for the remainder of the paper. Furthermore, we are restricted to the anisotropic case $0<\gamma\le 1$.

The off-diagonal correlation functions and the diagonal correlation functions, calculated in earlier papers by Niemeijer[3] and by McCoy, Barouch, and Abraham (MBA),[6] are the objects one needs to calculate in the linear response theory of Kubo.[7] Therefore, it is of interest to obtain exact results on such functions, even at zero temperature.

We study the off-diagonal correlation functions through the formalism of MBA. This formalism is a generalization of the method used by Cheng and Wu[8] in their study of the correlation functions of the two-dimensional Ising model. We extract the first-order term of $\rho_{xy}(R,t)$ for large R or t. Furthermore, we are able to obtain exact closed expressions for $\rho_{xz}(R,t)$ and $\rho_{yz}(R,t)$ in terms of contour integrals. We analyze these integrals for large R or t.

We find that as $R\to\infty$, $\rho_{xy}(R,t)$ goes to zero exponentially in R when $h\neq 1$. As $t\to\infty$, $\rho_{xy}(R,t)$ goes to zero as $t^{-1/2}$ for $h>1$ and t^{-1} for $h<1$. For $h<1$, $\rho_{xz}(R,t)$ has a nonzero limit for $R\to\infty$ or $t\to\infty$. The approach to this limit as a function of R or t large has the same character as the approach of $\rho_{xy}(R,t)$ to zero. $\rho_{xz}(R,t)$ for $h>1$ and $\rho_{yz}(R,t)$ for all h are identically zero.

II. SYMMETRY

As will be discussed later, it is difficult to calculate $\rho_{\mu\nu}(R,t)$ directly from (1.2). Therefore, we define

$$C_{\mu\nu}(R,t)=\langle S^\mu_{N/2+R}(0)S^\mu_N(0)S^\nu_R(t)S^\nu_{N/2}(t)\rangle \qquad (2.1)$$

and use the cluster property of $C_{\mu\nu}(R,t)$ as $N\to\infty$ to relate

$$\lim_{N\to\infty}\rho^2_{\mu\nu}(R,t)=\lim_{N\to\infty}C_{\mu\nu}(R,t)\ . \qquad (2.2)$$

The use of (2.2) to compute $\rho_{\mu\nu}$ for $N\to\infty$ is not completely equivalent to using (1.2). If we place magnetic fields on the system in the x and y directions, then (explicitly showing the dependence of $\rho_{\mu\nu}$ on h_x and h_y)

$$\lim_{h_x\to 0^\pm}\ \lim_{h_y\to 0^\pm}\ \lim_{N\to\infty}\ \rho^2_{\mu\nu}(R,t;h_x,h_y)=\lim_{N\to\infty}C_{\mu\nu}(R,t)\ . \qquad (2.3)$$

(If $h=0$, there will also be a h_z limit on the left-hand side.) One cannot arbitrarily change the order of limits on the left-hand side of (2.3). This is analogous to the small h_z needed in the two-dimensional Ising model to calculate the spontaneous magnetization $M(h_z)$ at $h_z=0$ by means of

$$\lim_{h_z\to 0^\pm}\ \lim_{N\to\infty}\ M^2(h_z)=\lim_{K\to\infty}\ \lim_{N\to\infty}\ \langle\sigma_{0,0}\,\sigma_{0,K}\rangle\ . \qquad (2.4)$$

Keeping the preceding discussion in mind, we present a symmetry operation and make an argument which is valid for all t and all temperature. The operation rotates the system 180° around the z axis and changes $h_x\to -h_x$ and $h_y\to -h_y$. The Hamiltonian transforms into itself and, therefore, for N finite any thermal average of spin operators should transform into itself. One obtains (deleting R and t dependences)

$$\rho_{xy}(h_x,h_y)=\rho_{xy}(-h_x,-h_y)\ , \qquad (2.5a)$$

$$\rho_{xz}(h_x,h_y)=-\rho_{xz}(-h_x,-h_y), \qquad (2.5b)$$

$$\rho_{yz}(h_x,h_y)=-\rho_{yz}(-h_x,-h_y)\ . \qquad (2.5c)$$

For N finite these functions are continuous in h_x and h_y, and, therefore, for $h_x=h_y=0$, $\rho_{xz}(R,t)=\rho_{yz}(R,t)=0$ for all t and all temperatures. If $N\to\infty$, the resulting functions are not necessarily continuous at $h_x=h_y=0$ and no rigorous conclusions can be reached. However, since there is never any long range order in the y direction, we believe all of the $\rho_{\mu\nu}(R,t)$ are continuous in h_y. There is long range order in the x direction only when $h<1$ and the temperature equals zero. Therefore, it is reasonable to expect $\lim_{N\to\infty}\rho_{xz}$ to be discontinuous and nonzero at $h_x=h_y=0^\pm$ for $h<1$ and zero temperature. We anticipate that $\lim_{N\to\infty}\rho_{yz}$, all $0\le h$, and $\lim_{N\to\infty}\rho_{xz}$, $1<h$, are zero for all temperatures. Later analytical work will verify the conjectures at zero temperature.

No conclusions can be reached about ρ_{xy} since it is even in both h_x and h_y.

One can also rotate about the x or y directions and find the evenness or oddness of the $\rho_{\mu\nu}$ as a function of h. From this we see that ρ_{xy} is an odd function of h, but there is no reason to assume that ρ_{xy} is continuous at $h=0$.

For the remainder of the paper we, in most instances, will not explicitly write the h_x and h_y limits even though when we take $N\to\infty$ on $\rho_{\mu\nu}$, they are implied.

III. FORMULATION AND $\rho_{xy}(R,t)$

The first step in an analysis of the X-Y model is to transform to Fermi creation and annihilation operators by the Jordan-Wigner transformation,[1]

$$c_k=\exp\left(\pi i\sum_1^{k-1}a_j a_j^\dagger\right)a_k\,. \tag{3.1}$$

One obtains

$$H=\frac{1}{2}\Big[\sum_1^{N-1}(c_j^\dagger c_{j+1}+c_{j+1}^\dagger c_j+\gamma c_j^\dagger c_{j+1}^\dagger+\gamma c_{j+1}c_j) -2h\sum_1^N(c_j^\dagger c_j-\tfrac{1}{2})-(c_N^\dagger c_1+c_1^\dagger c_N+\gamma c_N^\dagger c_1^\dagger+\gamma c_1 c_N)\times\exp\left(\pi i\sum_1^N c_j^\dagger c_j\right)\Big], \tag{3.2}$$

and if

$$A_i(t)=c_i^\dagger(t)+c_i(t)\,, \tag{3.3a}$$

$$B_i(t)=c_i(t)-c_i^\dagger(t)\,, \tag{3.3b}$$

then, one has

$$C_{xy}(R,t)=\pm\frac{1}{16}\left\langle\prod_{N/2+R}^{N-1}B_i(0)\prod_{N/2+R+1}^{N}A_j(0)\times{\prod_{N/2-1}^{R}}'A_k(t){\prod_{N/2}^{R+1}}'B_l(t)\right\rangle, \tag{3.4a}$$

$$C_{xx}(R,t)=\pm\frac{1}{16}\left\langle\prod_{N/2+R}^{N-1}B_i(0)\prod_{N/2+R+1}^{N}A_j(0)\times A_{N/2}(t)A_R(t)B_{N/2}(t)B_R(t)\right\rangle, \tag{3.4b}$$

$$C_{yx}(R,t)=\pm\frac{1}{16}\left\langle\prod_{N/2+R+1}^{N}B_i(0)\prod_{N/2+R}^{N-1}A_j(0)\times A_{N/2}(t)A_R(t)B_{N/2}(t)B_R(t)\right\rangle, \tag{3.4c}$$

where $\prod'$ indicates that the product runs from the larger limit to the smaller limit. The operator $\exp(\pi i\sum_1^N c_i^\dagger c_i)$ commutes with the Hamiltonian and has eigenvalues $P=\pm 1$. The ± 1 appearing in each expression for the $C_{\mu\nu}(R,t)$ can be determined but is irrelevant for our later discussion.

One is tempted to redefine the boundary condition on H so that it is cyclic in the c space. This was the procedure used in calculating the partition function[1] and time-independent correlation functions,[1,4,5] and, as one might suspect, it contributed errors of order N^{-1} to the results for these quantities. However, as indicated by MBA, one cannot proceed in this manner and obtain a correct result if one calculates $\rho_{\mu\nu}(R,t)$ from (1.2). Furthermore, because certain information about the exact eigenstates of H is not known to us, we are unable to use (1.2) with the correct boundary condition. However, one can make arguments which indicate that changing the boundary condition will not influence the results from $C_{\mu\nu}(R,t)$ to first order in N. Therefore, we choose $P=1$ for all states and proceed to use $C_{\mu\nu}(R,t)$ to obtain $\rho_{\mu\nu}(R,t)$.

To effect the diagonalization of H, we first perform the transformation

$$c_j=(e^{i\pi/4}/N^{1/2})\sum_{\phi_n}e^{-ij\phi_n}a_{\phi_n}\,, \tag{3.5}$$

where $\phi_n=\pm(\pi/N)(2n+1)$ with $n=0,1,\ldots,N/2-1$. Then we make a Bogoliubov transformation to Fermi creation and annihilation operators, $\eta_\phi^\dagger$ and η_ϕ, such that

$$a_\phi=\cos\theta_\phi\,\eta_\phi+\sin\theta_\phi\,\eta_{-\phi}^\dagger\,, \tag{3.6a}$$

$$a_{-\phi}=\cos\theta_\phi\,\eta_{-\phi}-\sin\theta_\phi\,\eta_\phi^\dagger\,, \tag{3.6b}$$

where

$$\tan 2\theta_\phi=\gamma\sin\phi/(\cos\phi-h)\,, \tag{3.6c}$$

with $0<\theta_\phi<\frac{1}{2}\pi$. We obtain

$$H=\sum_\phi\Lambda(\phi)\eta_\phi^\dagger\eta_\phi-\tfrac{1}{2}\sum_\phi\Lambda(\phi)\,, \tag{3.7a}$$

where

$$\Lambda(\phi)=[(\cos\phi-h)^2+\gamma^2\sin^2\phi]^{1/2}\,. \tag{3.7b}$$

The A's and B's of $C_{\mu\nu}(R,t)$ are expressible linearly in terms of $\eta_\phi^\dagger$ and η_ϕ. Therefore, using a generalization of the Wick theorem of quantum field theory,[1] one is able for arbitrary μ and ν to express $C_{\mu\nu}(R,t)$ as

$$C_{\mu\nu}(R,t)=\pm\tfrac{1}{16}\,Pf\,\Xi\,, \tag{3.8}$$

where $Pf\,\Xi$ is the Pfaffian of the antisymmetric matrix Ξ. The elements of Ξ consist of all possible contractions of the $A_i(t)$ and $B_i(t)$ factors (both $t=0$ and $t\neq 0$ factors) which appear in (3.4). The basic nonzero contractions which result are

$$\langle A_j(0)A_k(t)\rangle=-\langle B_j(0)B_k(t)\rangle=(1/N)\sum_\phi e^{i(k-j)\phi}e^{i\Lambda(\phi)t}\,, \tag{3.9a}$$

$$\langle A_j(0)B_k(t)\rangle=-(1/N)\sum_\phi e^{i\phi(j-k)}e^{i\Lambda(\phi)t}\Phi(\phi)\,, \tag{3.9b}$$

$$\langle B_j(0)A_k(t)\rangle=(1/N)\sum_\phi e^{i\phi(k-j)}e^{i\Lambda(\phi)t}\Phi(\phi)\,, \tag{3.9c}$$

where

$$\Phi(\phi) = e^{-i\phi}\left(\frac{(1-\lambda_1^{-1}e^{i\phi})(1-\lambda_2^{-1}e^{i\phi})}{(1-\lambda_1^{-1}e^{-i\phi})(1-\lambda_2^{-1}e^{-i\phi})}\right)^{1/2}, \tag{3.10a}$$

$$\lambda_1 = \frac{h+[h^2-1+\gamma^2]^{1/2}}{1-\gamma}, \tag{3.10b}$$

$$\lambda_2 = \frac{h-[h^2-1+\gamma^2]^{1/2}}{1-\gamma}. \tag{3.10c}$$

The square root defining $\Phi(\phi)$ is a positive number at $\phi=\pi$ and $\lambda_1(\lambda_2)$ has a positive (negative) imaginary part when $h<[1-\gamma^2]^{1/2}$.

We now calculate the $\rho_{\mu\nu}(R,t)$ and extract their behavior for large R and large t. First, we approach $\rho_{xy}(R,t)$:

$$C_{xy}(R,t) = \langle S^x_{N/2+R}(0)S^x_N(0)S^y_R(t)S^y_{N/2}(t)\rangle = \pm\tfrac{1}{16}\,Pf\,\Xi, \tag{3.11a}$$

with

$$\Xi = \begin{pmatrix} 0 & S & \Gamma & \Delta \\ -S^T & 0 & -E & -K \\ -\Gamma & E & 0 & -\hat{S} \\ -\Delta & K & \hat{S}^T & 0 \end{pmatrix}, \tag{3.11b}$$

where

$$S_{m,n} = (1/N)\textstyle\sum_\phi \Phi(\phi)\,e^{i\phi(n-m+1)}, \tag{3.11c}$$

$$\hat{S}_{m,n} = (1/N)\textstyle\sum_\phi \Phi(\phi)\,e^{i\phi(n-m-1)}, \tag{3.11d}$$

$$\Gamma_{m,n} = (1/N)\textstyle\sum_\phi e^{i\Lambda(\phi)t}\,\Phi(\phi)\,e^{-i\phi(n+m+1+R)}, \tag{3.11e}$$

$$K_{m,n} = (1/N)\textstyle\sum_\phi e^{i\Lambda(\phi)t}\,\Phi(\phi)\,e^{i\phi(n+m+1+R)}, \tag{3.11f}$$

$$\Delta_{m,n} = -(1/N)\textstyle\sum_\phi e^{i\Lambda(\phi)t}\,e^{i\phi(n+m+R)}, \tag{3.11g}$$

$$E_{m,n} = -(1/N)\textstyle\sum_\phi e^{i\Lambda(\phi)t}\,e^{i\phi(n+m+R+2)} \tag{3.11h}$$

for $m, n = 0, 1, \ldots, N/2-R-1$. The analysis of Ξ must now separate into three cases, $h<1$, $h>1$, and $h=1$, since the character of $\Phi(\phi)$ is different in each region. We cannot treat the last case but continue the procedure of MBA for the first two cases.

A. $h>1$, $|\lambda_1|>1$, and $|\lambda_2^{-1}|>1$

Define a new matrix Ω such that

$$\Omega = \begin{pmatrix} \underline{0}| & |\underline{S} & |\underline{\Gamma} & \underline{\Delta}| \\ -\overline{S^T}| & |\overline{0} & |-\overline{E} & -\overline{K}| \\ -\overline{\Gamma}| & |\overline{E} & |\overline{0} & -\overline{\hat{S}}| \\ -\underline{\Delta}| & |\underline{K} & |\underline{\hat{S}^T} & \underline{0}| \end{pmatrix}$$

$$= \begin{pmatrix} 0 & \tilde{S} & \tilde{\Gamma} & \tilde{\Delta} \\ -\tilde{S}^T & 0 & -\tilde{\Delta} & -\tilde{K} \\ -\tilde{\Gamma} & \tilde{\Delta} & 0 & -\tilde{S} \\ -\tilde{\Delta} & \tilde{K} & \tilde{S}^T & 0 \end{pmatrix}, \tag{3.12a}$$

where

$$\tilde{S}_{m,n} = (1/N)\textstyle\sum_\phi \Phi(\phi)\,e^{i\phi(n-m)}, \tag{3.12b}$$

$$\tilde{\Gamma}_{m,n} = (1/N)\textstyle\sum_\phi e^{i\Lambda(\phi)t}\,\Phi(\phi)\,e^{-i\phi(n+m+R)}, \tag{3.12c}$$

$$\tilde{K}_{m,n} = (1/N)\textstyle\sum_\phi e^{i\Lambda(\phi)t}\,\Phi(\phi)\,e^{i\phi(n+m+R)}, \tag{3.12d}$$

$$\tilde{\Delta}_{m,n} = -(1/N)\textstyle\sum_\phi e^{i\Lambda(\phi)t}\,e^{i\phi(n+m+R)}, \tag{3.12e}$$

with $m, n = 0, \ldots, N/2-R$. The horizontal (vertical) lines indicate rows (columns) added to Ξ to obtain Ω.

For the next step and some later parts of the calculation, we need to know some of the general characteristics of the submatrices that comprise Ω. (The characteristics of the corresponding submatrices of Ξ are the same.) One notes that $\tilde{S}$ is Toeplitz and, therefore, has constant matrix elements along its diagonal and any lines parallel to its diagonal. For N large as one goes away from the diagonal, the matrix elements decrease exponentially in the distance from the diagonal. $\tilde{\Gamma}$, $\tilde{K}$, and $\tilde{\Delta}$ are not Toeplitz but, instead, have constant matrix elements along lines perpendicular to the diagonal. For R and t fixed but N large, the larger elements of these three submatrices are in the upper left-hand corner ($m, n=0$ region) and in the lower right-hand corner ($m, n=N/2-R$ region). As one goes away from either region, the matrix elements fall off exponentially until one reaches the centers of the matrices. If one allows R to become large, but not of order N, each matrix element of $\tilde{\Gamma}$, $\tilde{K}$, and $\tilde{\Delta}$ becomes exponentially small in R. If t becomes large, each element goes to zero as $t^{-1/2}$.

We use the last two statements of the preceding paragraph to find that as $R\to\infty$ or $t\to\infty$

$$\lim_{N\to\infty}\det\Omega \to \left(\lim_{N\to\infty}\tilde{S}\right)^4. \tag{3.13}$$

Since $\tilde{S}$ is Toeplitz, one can use Szegö's theorem[9] to find that

$$\lim_{N\to\infty}\det\tilde{S} = \left(\frac{(\lambda_2-\lambda_2^{-1})(\lambda_1^{-1}-\lambda_1)}{(\lambda_2-\lambda_1)(\lambda_1^{-1}-\lambda_2^{-1})}\right)^{1/4}. \tag{3.14}$$

We now need the ratio (valid for finite N)

$$s^2 = \det\Xi/\det\Omega. \tag{3.15}$$

Using Jacobi's theorem[10] for the expansion of a determinant, one can show that if one has two matrices α and β, where β is obtained from α by the deletion of rows and columns in positions $l_1, l_2, \ldots, l_k$, then

$$\frac{\det\beta}{\det\alpha}=\det\begin{pmatrix}(\alpha^{-1})_{l_1,l_1} & (\alpha^{-1})_{l_1,l_2} & \cdots (\alpha^{-1})_{l_1,l_k}\\ (\alpha^{-1})_{l_2,l_1} & (\alpha^{-1})_{l_2,l_2} & \cdot\\ \vdots & & \vdots\\ (\alpha^{-1})_{l_k,l_1} & \cdots & (\alpha^{-1})_{l_k,l_k}\end{pmatrix} \tag{3.16}$$

Since Ω and, correspondingly, Ω^{-1} are antisymmetric, the small matrix giving s^2 is antisymmetric. Therefore, using the relation between Pfaffians and determinants and (3.16), one obtains

$$s^2=[(\Omega^{-1})_{l_1,l_2}(\Omega^{-1})_{l_3,l_4}-(\Omega^{-1})_{l_1,l_3}(\Omega^{-1})_{l_2,l_4}+(\Omega^{-1})_{l_1,l_4}(\Omega^{-1})_{l_2,l_3}]^2\,, \tag{3.17}$$

where l_1, l_2, l_3, and l_4 are the rows and columns one must delete from Ω to obtain Ξ.

To obtain Ω^{-1}, we make use of the smallness of $\tilde\Gamma$, $\tilde\Delta$, and $\tilde K$ for R or t large and perform a series expansion of Ω^{-1} in terms of them. Exhibiting the first two terms,

$$\Omega^{-1}=\begin{pmatrix}\underline{0}| & |-(\tilde S^T)^{-1} & |-(\tilde S^T)^{-1}\tilde K\tilde S^{-1} & (\tilde S^T)^{-1}\tilde\Delta(\tilde S^T)^{-1}|\\ \bar{\tilde S}^{-1} & 0 & -\tilde S^{-1}\tilde\Delta\tilde S^{-1} & \tilde S^{-1}\tilde\Gamma(\tilde S^T)^{-1}\\ (\bar{\tilde S}^T)^{-1}\tilde K\tilde S^{-1} & (\tilde S^T)^{-1}\tilde\Delta(\tilde S^T)^{-1} & 0 & (\tilde S^T)^{-1}\\ -\underline{\tilde S}^{-1}\tilde\Delta\tilde S^{-1} & -\tilde S^{-1}\tilde\Gamma(\tilde S^T)^{-1} & -\tilde S^{-1} & 0\end{pmatrix}+\cdots\,, \tag{3.18}$$

where the horizontal (vertical) lines indicate the positions of rows (columns) l_1, l_2, l_3, and l_4.

By examining the equation $\tilde S\tilde S^{-1}=1$, one is able to see that the matrix elements of $\tilde S^{-1}$ decrease exponentially away from its diagonal. This implies that $(\Omega^{-1})_{l_1,l_2}$ and $(\Omega^{-1})_{l_3,l_4}$ are exponentially small in N and go to zero in the thermodynamic limit. By combining the characteristics of $\tilde\Gamma$, $\tilde K$, and $\tilde\Delta$ with those of $\tilde S^{-1}$ to get the characteristics of their products, we see that $(\Omega^{-1})_{l_1,l_3}$ and $(\Omega^{-1})_{l_2,l_4}$ are also exponentially small in N. Therefore, for large N

$$s^2\sim\{[\tilde S^{-1}\tilde\Delta\tilde S^{-1}]_{0,0}[(\tilde S^T)^{-1}\tilde\Delta(\tilde S^T)^{-1}]_{N/2-R,N/2-R}\}^2+\cdots\,. \tag{3.19}$$

But by inverting all sums in the matrix products in the second factor, we can prove equality between the two factors for N, R, and t finite. Finally,

$$s^2\sim[(\tilde S^{-1}\tilde\Delta\tilde S^{-1})_{0,0}]^4+\cdots\,. \tag{3.20}$$

One obtains $\tilde S^{-1}$ for $N\to\infty$ from the Wiener-Hopf equation

$$\sum_{l=0}^{\infty}\tilde S_{m,l}(\tilde S^{-1})_{l,n}=\delta_{m,n}\,,\quad 0\le m,n\,. \tag{3.21}$$

This yields

$$\lim_{N\to\infty}(\tilde S^{-1})_{m,n}=\frac{1}{(2\pi)^2}\oint d\xi\,\xi^{-m-1}\left(\frac{\lambda_2^{-1}-\xi}{1-\lambda_1^{-1}\xi}\right)^{1/2}\times\oint d\xi'\,\frac{1}{\xi'-\xi}\,\xi'^{\,n}\left(\frac{\lambda_1^{-1}-\xi'}{1-\lambda_2^{-1}\xi'}\right)^{1/2}, \tag{3.22}$$

where $|\xi|=1$ and $|\xi'|=1+\epsilon>1$. Using (3.22) and (3.12e) with $N\to\infty$

$$\lim_{N\to\infty}s^2=\left(\frac{1}{2\pi i}\oint dz\,z^{R-1}e^{it\Lambda(z)}\right)^4+\cdots\,, \tag{3.23}$$

where

$$\Lambda(z)=\frac{(1-\gamma^2)^{1/2}}{2z}[(z-\lambda_1)(z-\lambda_2)(z-\lambda_1^{-1})(z-\lambda_2^{-1})]^{1/2}\,.$$

[Note that $\Lambda(z)=\Lambda(\phi)$ for $z=e^{i\phi}$.] The contour is $|z|=1$. The first term in (3.23) gives the first-order contribution to s^2 for R or t large.

Therefore, we obtain for R or t large

$$\lim_{N\to\infty}\rho_{xy}(R,t)\sim\frac{\eta}{4}\left(\frac{(\lambda_2-\lambda_2^{-1})(\lambda_1^{-1}-\lambda_1)}{(\lambda_2-\lambda_1)(\lambda_1^{-1}-\lambda_2^{-1})}\right)^{1/4}\times\left(\frac{1}{2\pi i}\oint dz\,z^{R-1}e^{it\Lambda(z)}\right)\,, \tag{3.24}$$

where $\eta=\pm1$, $\pm i$ is a phase factor arising from the fourth root taken in obtaining ρ_{xy} and depends on whether $h_x\to0^+$ or 0^-.

For t large and R fixed the integral remains on the unit circle contour and stationary phase used to obtain the large t behavior. For large R and fixed t the contour is contracted to one around the cut inside the unit circle and the method of Laplace is applied to extract the large R dependence. One obtains

(a) $t\to\infty$, $h>1$:

$$\lim_{N\to\infty}\rho_{xy}(R,t)\sim\frac{\eta}{4(2\pi t)^{1/2}}\left(\frac{(\lambda_2-\lambda_2^{-1})(\lambda_1^{-1}-\lambda_1)}{(\lambda_2-\lambda_1)(\lambda_1^{-1}-\lambda_2^{-1})}\right)^{1/4}$$

$$\times\left[\exp\!\left(i\,\frac{\pi}{4}+it(h-1)\right)\left(\frac{h-1}{\gamma^2-1+h}\right)^{1/2}\right.$$
$$\left.+(-1)^R\exp\!\left(-i\,\frac{\pi}{4}+it(h+1)\right)\left(\frac{h+1}{h+1-\gamma^2}\right)^{1/2}\right]; \qquad (3.25)$$

(b) $R\to\infty,\ h>1$:

$$\lim_{N\to\infty}\rho_{xy}(R,t)\sim\frac{\eta t\lambda_2^{R-1/2}}{4(2\pi)^{1/2}R^{3/2}}\left(\frac{(\lambda_2-\lambda_2^{-1})(\lambda_1^{-1}-\lambda_1)}{(\lambda_2-\lambda_1)(\lambda_1^{-1}-\lambda_2^{-1})}\right)^{1/4}$$
$$\times[h^2-1+\gamma^2]^{1/2}\left(\frac{\gamma\lambda_2}{1+\gamma}\right)^{1/2}. \qquad (3.26)$$

B. $h<1$, $|\lambda_1|>1$, and $|\lambda_2|>1$

We cannot proceed in the same fashion as for $h>1$ since the properties of $\Phi(\phi)$ have changed, rendering invalid the use of Szegö's theorem to obtain $\det\bar{S}$ and the procedure to find $\bar{S}^{-1}$. In particular, for $h>1$

$$\ln\Phi(0)-\ln\Phi(2\pi)=0\ , \qquad (3.27)$$

but not for $h<1$. Therefore, we must select a different matrix. Take

$$\Omega_1=\begin{pmatrix} |\underline{0}| & |\underline{S}| & ||\underline{\Gamma} & \underline{\Delta}|| \\ |-\underline{S}^T| & |\underline{0}| & ||-\underline{E} & -\underline{K}|| \\ |-\overline{\overline{\Gamma}}| & |\overline{\overline{E}}| & ||\overline{\overline{0}} & -\overline{\overline{S}}|| \\ |-\underline{\underline{\Delta}}| & |\underline{\underline{K}}| & ||\underline{\underline{\hat{S}^T}} & \underline{\underline{0}}|| \end{pmatrix}$$

$$=\begin{pmatrix} 0 & \bar{S} & \bar{\Gamma} & \bar{\Delta} \\ -\bar{S}^T & 0 & -\bar{\Delta} & -\bar{K} \\ -\bar{\Gamma} & \bar{\Delta} & 0 & -\bar{S} \\ -\bar{\Delta} & \bar{K} & \bar{S}^T & 0 \end{pmatrix}, \qquad (3.28a)$$

where

$$\bar{S}_{m,n}=(1/N)\textstyle\sum_\phi \Phi(\phi)\,e^{i\phi(n-m+1)}\ , \qquad (3.28b)$$

$$\bar{\Gamma}_{m,n}=(1/N)\textstyle\sum_\phi e^{i\Lambda(\phi)t}\Phi(\phi)\,e^{-i\phi(n+m+R-2)}\ , \qquad (3.28c)$$

$$\bar{\Delta}_{m,n}=-(1/N)\textstyle\sum_\phi e^{i\Lambda(\phi)t}\,e^{i\phi(n+m+R-1)}\ , \qquad (3.28d)$$

$$\bar{K}_{m,n}=(1/N)\textstyle\sum_\phi e^{i\Lambda(\phi)t}\,\Phi(\phi)\,e^{i\phi(n+m+R)}\ , \qquad (3.28e)$$

with $m,n=0,\ \ldots,\ N/2-R+1$. The horizontal (vertical) lines indicate added rows (columns).

The extra factor of $e^{i\phi}$ in the definition of $\bar{S}_{m,n}$ combined with $\Phi(\phi)$ forms a function which satisfies (3.27) for $h<1$, making it possible to find $\det\bar{S}$ by Szegö's theorem and $\bar{S}^{-1}$ from the Wiener-Hopf equation. Therefore, we proceed in the same manner as for $h>1$.

We have that

$$s_1^2=\det\Xi/\det\Omega_1 \qquad (3.29)$$

is equal to the determinant of an 8×8 matrix consisting of certain matrix elements of Ω_1^{-1}. Again one can show that some matrix elements are equal and, using the character of the submatrices of Ω_1, that others are exponentially small in N. After evaluating the remaining elements of the 8×8 matrix for $N\to\infty$, one finds that to first order in R or t

$$\lim_{N\to\infty}s_1^2\sim\frac{(1+\gamma)^4}{16}\left[\left(\frac{1}{2\pi i}\oint dz\,e^{i\Lambda(z)t}z^{R-2}\right)\right.$$
$$\times\left(\frac{1}{2\pi i}\oint dz\,\frac{e^{i\Lambda(z)t}z^{R-1}}{\Lambda(z)}\right)-\left(\frac{1}{2\pi i}\oint dz\,e^{i\Lambda(z)t}z^{R-1}\right)$$
$$\left.\times\left(\frac{1}{2\pi i}\oint dz\,\frac{e^{i\Lambda(z)t}z^{R-2}}{\Lambda(z)}\right)\right]^4. \qquad (3.30)$$

Furthermore, to first order in R or t

$$\lim_{N\to\infty}\det\Omega_1\sim\frac{16\gamma^2(1-h^2)}{(1+\gamma)^4}\ , \qquad (3.31)$$

and, therefore,

$$\lim_{N\to\infty}\rho_{xy}(R,t)\sim\frac{\eta\gamma^{1/2}(1-h^2)^{1/4}}{2(1+\gamma)}\lim_{N\to\infty}s_1^{1/2}\ , \qquad (3.32)$$

where $\lim_{N\to\infty}s_1^{1/2}$ is given by (3.30).

Further analysis of s_1^2 is more difficult than that for s^2 with $h>1$. In the stationary phase computation $h<1$ splits into two regions, $h\gtrless1-\gamma^2$, with two stationary phase points (same as for $h>1$) for $h>1-\gamma^2$ and four points for $h<1-\gamma^2$. If $h>[1-\gamma^2]^{1/2}$ in the large R computation, λ_1^{-1} and λ_2^{-1} are real and the cut inside the unit circle is on the real axis. However, for $h<[1-\gamma^2]^{1/2}$, λ_1^{-1} and λ_2^{-1} are complex conjugates of each other and a modification of the contour and the analysis is needed. In performing the calculations one finds

(a) $t\to\infty,\ 1-\gamma^2<h<1$:

$$\lim_{N\to\infty}\rho_{xy}(R,t)\sim\frac{\eta h e^{2it}}{2\pi t}\,\frac{\gamma^{1/2}(1-h^2)^{1/4}}{[(1-h^2)(1+h-\gamma^2)(\gamma^2-1+h)]^{1/2}}\,; \qquad (3.33)$$

(b) $t\to\infty,\ 0\le h<1-\gamma^2$:

$$\lim_{N\to\infty}\rho_{xy}(R,t)\sim\frac{\eta\gamma^{1/2}(1-h^2)^{1/4}}{8\pi t}$$
$$\times\left[\frac{(-1)^R\,4hi\,e^{2it}}{[(1-h^2)(1-h-\gamma^2)(1+h-\gamma^2)]^{1/2}}\right.$$
$$+\frac{e^{it(1-h+\Lambda_0)}}{(\Lambda_0'')^{1/2}}\left(\frac{1-h}{1-h-\gamma^2}\right)^{1/2}\left(\frac{1}{\Lambda_0}-\frac{1}{1-h}\right)$$

$$\times[z_0^{R-1}(z_0-1)+z_0^{*R-1}(z_0^*-1)]$$

$$+\frac{(-1)^{R-1}e^{it(1+h+\Lambda_0)}}{(\Lambda_0'')^{1/2}}\left(\frac{1+h}{1+h-\gamma^2}\right)^{1/2}\left(\frac{1}{\Lambda_0}-\frac{1}{1+h}\right)$$

$$\times[z_0^{R-1}(z_0+1)+z_0^{*R-1}(z_0^*+1)]\Bigg] , \quad (3.34a)$$

where

$$\Lambda_0''=\frac{(1-\gamma^2)^2-h^2}{\gamma}[(1-\gamma^2)(1-\gamma^2-h^2)]^{-1/2} , \quad (3.34b)$$

$$\Lambda_0=\gamma[(1-\gamma^2-h^2)/(1-\gamma^2)]^{1/2} , \quad (3.34c)$$

$$z_0=\frac{h}{1-\gamma^2}+i\frac{[(1-\gamma^2)^2-h^2]^{1/2}}{1-\gamma^2} ; \quad (3.34d)$$

(c) $R\to\infty$, $(1-\gamma^2)^{1/2}<h<1$:

$$\lim_{N\to\infty}\rho_{xy}(R,t)\sim\frac{\eta\gamma^{1/2}(1-h^2)^{1/4}t\lambda_2}{8\pi R^3\lambda_2^{2R}} ; \quad (3.35)$$

(d) $R\to\infty$, $0\le h<[1-\gamma^2]^{1/2}$:

$$\lim_{N\to\infty}\rho_{xy}(R,t)\sim\frac{\eta\gamma^{1/2}[1-h^2]^{1/4}t\rho_0^{2R-1}\cos(\alpha_0/\gamma)}{2\pi R^2(1-\gamma^2)}$$

$$\times[1-\gamma^2-h^2]^{1/2} , \quad (3.36a)$$

where

$$\rho_0=[(1-\gamma)/(1+\gamma)]^{1/2} , \quad (3.36b)$$

$$\alpha_0=\tan^{-1}[(1-\gamma^2-h^2)^{1/2}/h] . \quad (3.36c)$$

Again $\eta=\pm1$, $\pm i$ and depends on whether $h_x\to0^+$ or 0^-.

IV. $\rho_{xz}(R,t)$ AND $\rho_{yz}(R,t)$

For $\rho_{xz}(R,t)$ we have

$$C_{xz}(R,t)=\langle S^x_{N/2+R}(0)S^x_N(0)S^z_R(t)S^z_{N/2}(t)\rangle=\pm\tfrac{1}{16}\,Pf\,\Xi \quad (4.1a)$$

for

$$\Xi=\begin{pmatrix} 0 & S & \Gamma^1 & \Gamma^2 & \Delta^1 & \Delta^2 \\ -S^T & 0 & -E^1 & -E^2 & -K^1 & -K^2 \\ -\Gamma^{1T} & E^{1T} & 0 & 0 & -S_{1,0} & -S_{1,N/2-R} \\ -\Gamma^{2T} & E^{2T} & 0 & 0 & -S_{N/2-R+1,0} & -S_{1,0} \\ -\Delta^{1T} & K^{1T} & S_{1,0} & S_{N/2-R+1,0} & 0 & 0 \\ -\Delta^{2T} & K^{2T} & S_{1,N/2-R} & S_{1,0} & 0 & 0 \end{pmatrix} , \quad (4.1b)$$

where

$$S_{m,n}=(1/N)\textstyle\sum_\phi \Phi(\phi)e^{i\phi(n-m+1)} , \quad (4.1c)$$

$$\Gamma^j_m=(1/N)\textstyle\sum_\phi e^{i\Lambda(\phi)t}\Phi(\phi)e^{-i\phi(m+\alpha_j)} , \quad (4.1d)$$

$$\Delta^j_m=-(1/N)\textstyle\sum_\phi e^{i\Lambda(\phi)t}e^{-i\phi(m+\alpha_j)} , \quad (4.1e)$$

$$E^j_m=-(1/N)\textstyle\sum_\phi e^{i\Lambda(\phi)t}e^{-i\phi(m+\alpha_j+1)} , \quad (4.1f)$$

$$K^j_m=(1/N)\textstyle\sum_\phi e^{i\Lambda(\phi)t}\Phi(\phi)e^{i\phi(m+\alpha_j+1)} , \quad (4.1g)$$

with $m,n=0,\ldots,N/2-R-1$. Also, $\alpha_1=R$ and $\alpha_2=N/2$. Note that $\Gamma^{1,2}$, $\Delta^{1,2}$, $E^{1,2}$, and $K^{1,2}$ are column vectors such that if the superscript is 1, the components decrease exponentially as m increases and if the superscript is 2, the components decrease exponentially as m decreases from $N/2-R-1$. Also, in the 4×4 submatrix we can drop the four elements which depend on $(N/2)$ since they go to zero as $N\to\infty$.

A. $h<1$, $|\lambda_1|>1$, and $|\lambda_2|>1$

One forms the ratio

$$s^2=\det\Omega/\det\Xi , \quad (4.2a)$$

where

$$\Omega=\begin{pmatrix}0 & S\\ -S^T & 0\end{pmatrix} . \quad (4.2b)$$

To facilitate the study of Ξ^{-1}, we introduce

$$U=\begin{pmatrix} 0 & -(S^T)^{-1} & & & & \\ S^{-1} & 0 & & & 0 & \\ & & 0 & 0 & (S_{1,0})^{-1} & 0 \\ & & 0 & 0 & 0 & (S_{1,0})^{-1} \\ & 0 & -(S_{1,0})^{-1} & 0 & 0 & 0 \\ & & 0 & -(S_{1,0})^{-1} & 0 & 0 \end{pmatrix} , \quad (4.3a)$$

and

$$V=\begin{pmatrix} & 0 & \Gamma^1 & \Gamma^2 & \Delta^1 & \Delta^2 \\ & & -E^1 & -E^2 & -K^1 & -K^2 \\ -\Gamma^{1T} & E^{1T} & & & & \\ -\Gamma^{2T} & E^{2T} & & & & \\ -\Delta^{1T} & K^{1T} & & 0 & & \\ -\Delta^{2T} & K^{2T} & & & & \end{pmatrix}. \tag{4.3b}$$

Then, we have

$$\Xi^{-1}=U\sum_{k=0}^{\infty}(-1)^k\,(VU)^k\,. \tag{4.4}$$

We are interested in the determinant of the 4×4 submatrix in the lower right-hand corner of Ξ^{-1}. By explicit calculation one finds that VU is zero in the 4×4 block. $(VU)^2$ is of the form

$$(VU)^2=\begin{pmatrix} ? & & 0 & & \\ & A & & 0 & \\ & & A & & \\ 0 & & & A & \\ & 0 & & & A \end{pmatrix}, \tag{4.5}$$

where we have made use of the characteristics of S^{-1}, $\Gamma^{1,2}$, $\Delta^{1,2}$, $E^{1,2}$, and $K^{1,2}$ to drop elements in the 4×4 block that are exponentially small in N. From the above information one sees that in the 4×4 block all odd powers of UV are zero and even powers are equal to A^k times the identity matrix. Therefore, we have

$$\lim_{N\to\infty}\Xi^{-1}_{4\times 4}=\lim_{N\to\infty}\frac{1}{1-A}\times\begin{pmatrix} 0 & 0 & (S_{1,0})^{-1} & 0 \\ 0 & 0 & 0 & (S_{1,0})^{-1} \\ -(S_{1,0})^{-1} & 0 & 0 & 0 \\ 0 & -(S_{1,0})^{-1} & 0 & 0 \end{pmatrix}, \tag{4.6}$$

and

$$\lim_{N\to\infty}s^2=\lim_{N\to\infty}(S_{1,0})^{-4}(1-A)^{-4}\,. \tag{4.7}$$

A is obtained from the calculation of $(VU)^2$. Then, we have

$$\lim_{N\to\infty}A=\lim_{N\to\infty}(S_{1,0})^{-1}[K^{1T}S^{-1}\Gamma^1-E^{1T}S^{-1}\Delta^1]$$

$$=\lim_{N\to\infty}(S_{1,0})^{-1}\Bigg[\left(\frac{1}{2\pi i}\oint dz\,e^{i\Lambda(z)t}z^{-R}[(1-\lambda_1^{-1}z)(1-\lambda_2^{-1}z)]^{-1/2}\frac{1}{2\pi i}\oint dz'\frac{e^{i\Lambda(z')t}z'^{-R-1}}{z'z-1+\epsilon}[(1-\lambda_1^{-1}z')(1-\lambda_2^{-1}z')]^{1/2}\right)$$

$$-\left(\frac{1}{2\pi i}\oint dz\,e^{i\Lambda(z)t}z^{R}[(1-\lambda_1^{-1}z)(1-\lambda_2^{-1}z)]^{-1/2}\frac{1}{2\pi i}\oint dz'\frac{e^{i\Lambda(z')t}z'^{R-1}}{1+\epsilon-zz'}[(1-\lambda_1^{-1}z')(1-\lambda_2^{-1}z')]^{1/2}\right)\Bigg], \tag{4.8a}$$

where

$$\lim_{N\to\infty}S_{1,0}=\frac{1}{2\pi i}\oint dz\,z^{-2}\left(\frac{(1-\lambda_1^{-1}z)(1-\lambda_2^{-1}z)}{(1-\lambda_1^{-1}z^{-1})(1-\lambda_2^{-1}z^{-1})}\right)^{1/2}. \tag{4.8b}$$

All contours are taken on the unit circle.

Using Szegö's theorem

$$\det\Omega=\frac{4\gamma[1-h^2]^{1/2}}{(1+\gamma)^2} \tag{4.9}$$

for $N\to\infty$.

All the above calculations for ρ_{xz} are exact for all values of R and t with $N\to\infty$. From them

$$\lim_{N\to\infty}\rho_{xz}(R,t)=\frac{\eta}{4}\frac{2^{1/2}\gamma^{1/4}}{(1+\gamma)^{1/2}}(1-h^2)^{1/8}\lim_{N\to\infty}S_{1,0}(1-A)\,, \tag{4.10}$$

where A and $S_{1,0}$ are given by (4.8).

One sees from (4.10) that there is long-range order in ρ_{xz}, and, therefore, one can use the $R\to\infty$ limit to partially determine η. In this limit we expect

$$\lim_{R\to\infty}\lim_{N\to\infty}\rho_{xz}(R,t)=\lim_{h_x\to 0\pm}\lim_{N\to\infty}\langle S^x{}_1\rangle\,\langle S^z{}_1\rangle\,. \tag{4.11}$$

It is a straightforward calculation to get

$$\langle S_1^z\rangle=\tfrac{1}{2}S_{1,0}\,. \tag{4.12}$$

We extract $\lim_{h_x\to 0\pm}\lim_{N\to\infty}\langle S^x{}_1\rangle$ from

$$\lim_{h_x\to 0\pm}\lim_{N\to\infty}\langle S_1^x\rangle^2=\lim_{R\to\infty}\lim_{N\to\infty}\langle S_1^xS_R^x\rangle$$

$$=\tfrac{1}{2}(1+\gamma)^{-1}\gamma^{1/2}[1-h^2]^{1/4}\,. \tag{4.13}$$

Therefore, we have $\eta=\xi\equiv\pm 1$. The ambiguity in ξ arises because h_x can be 0^+ or 0^-. (Note that we cannot apply this same method to determine η for ρ_{xy} because ρ_{xy} has no long-range order.)

One obtains the large R and t behavior of $\rho_{xz}(R,t)$ for $h<1$ in the same manner as for $\rho_{xy}(R,t)$,

$h<1$. We have

(a) $t\to\infty$, $1-\gamma^2<h<1$:

$$\lim_{N\to\infty} A \sim \frac{1}{2\pi S_{1,0}t}\left(\frac{(-1)^R\, 2i(\lambda_1^{-1}+\lambda_2^{-1})\,e^{2it}[1-h^2]^{1/2}}{[(1-\gamma^2-h)(1+h-\gamma^2)(1-\lambda_1^{-2})(1-\lambda_2^{-2})]^{1/2}} + \frac{(-1)^R\,(z_0^R+z_0^{*R})\exp it(\Lambda_0+1+h)}{(\Lambda''_0)^{1/2}}\left(\frac{1+h}{1+h-\gamma^2}\right)^{1/2}\right.$$

$$\times\left\{\frac{1}{z_0^*+1}\left[\left(\frac{(1-\lambda_1^{-1}z_0^*)(1-\lambda_2^{-1}z_0^*)}{(1+\lambda_1^{-1})(1+\lambda_2^{-1})}\right)^{1/2}-\left(\frac{(1+\lambda_1^{-1})(1+\lambda_2^{-1})}{(1-\lambda_1^{-1}z_0)\,(1-\lambda_2^{-1}z_0)}\right)^{1/2}\right]\right.$$

$$\left.+\frac{1}{z_0+1}\left[\left(\frac{(1-\lambda_1^{-1}z_0)(1-\lambda_2^{-1}z_0)}{(1+\lambda_1^{-1})(1+\lambda_2^{-1})}\right)^{1/2}-\left(\frac{(1+\lambda_1^{-1})\,(1+\lambda_2^{-1})}{(1-\lambda_1^{-1}z_0^*)(1-\lambda_2^{-1}z_0^*)}\right)^{1/2}\right]\right\}$$

$$+\frac{(z_0^R+z_0^{*R})\exp it(\Lambda_0+1-h)}{(\Lambda_0'')^{1/2}}\left(\frac{1-h}{1-\gamma^2-h}\right)^{1/2}\left\{\frac{1}{z_0^*-1}\left[\left(\frac{(1-\lambda_1^{-1}z_0^*)(1-\lambda_2^{-1}z_0^*)}{(1-\lambda_1^{-1})(1-\lambda_2^{-1})}\right)^{1/2}-\left(\frac{(1-\lambda_1^{-1})(1-\lambda_2^{-1})}{(1-\lambda_1^{-1}z_0)(1-\lambda_2^{-1}z_0)}\right)^{1/2}\right]\right.$$

$$\left.\left.+\frac{1}{z_0-1}\left[\left(\frac{(1-\lambda_1^{-1}z_0)(1-\lambda_2^{-1}z_0)}{(1-\lambda_1^{-1})(1-\lambda_2^{-1})}\right)^{1/2}-\left(\frac{(1-\lambda_1^{-1})(1-\lambda_2^{-1})}{(1-\lambda_1^{-1}z_0^*)(1-\lambda_2^{-1}z_0^*)}\right)^{1/2}\right]\right\}\right), \tag{4.15a}$$

where

$$\Lambda_0''=\frac{(1-\gamma^2)^2-h^2}{\gamma}\,[(1-\gamma^2)(1-\gamma^2-h^2)]^{-1/2}, \tag{4.15b}$$

$$\Lambda_0=\gamma[(1-\gamma^2-h^2)/(1-\gamma^2)]^{1/2}, \tag{4.15c}$$

$$z_0=\frac{h}{1-\gamma^2}+i\frac{[(1-\gamma^2)^2-h^2]^{1/2}}{1-\gamma^2}. \tag{4.15d}$$

The square roots are defined such that $[(1-\lambda_1^{-1}z)\times(1-\lambda_2^{-1}z)]^{1/2}$ is positive at $z=-1$.

(c) $R\to\infty$, $[1-\gamma^2]^{1/2}<h<1$:

$$\lim_{N\to\infty} A\sim-[2\pi S_{1,0}\lambda_2^{2R+1}R^2(1-\lambda_2^{-2})]^{-1}; \tag{4.16}$$

(d) $R\to\infty$, $0\le h<[1-\gamma^2]^{1/2}$:

$$\lim_{N\to\infty} A\sim-\frac{1}{2\pi S_{1,0}}\,\frac{\rho_0^{2R-1}}{R^2}\left(\frac{e^{i\alpha_0(2R-1)}}{\lambda_2^2-1}+\frac{e^{-i\alpha_0(2R-1)}}{\lambda_2^{*2}-1}\right), \tag{4.17a}$$

where

$$\rho_0=[(1-\gamma)/(1+\gamma)]^{1/2}, \tag{4.17b}$$

$$\alpha_0=\tan^{-1}[(1-\gamma^2-h^2)^{1/2}/h], \tag{4.17c}$$

$$\lambda_2=\frac{h-i[1-\gamma^2-h^2]^{1/2}}{1-\gamma}. \tag{4.17d}$$

As we mentioned earlier, the equilibrium correlation function $\rho_{xx}(R,0)$ has not been previously computed. Therefore, we include it here,

$$\lim_{N\to\infty} A\sim\frac{(-1)^{R+1}h\,e^{2it}}{S_{1,0}\pi t}\,[(h+1-\gamma^2)(\gamma^2-1+h)]^{-1/2}; \tag{4.14}$$

(b) $t\to\infty$, $0\le h<1-\gamma^2$:

$$\lim_{N\to\infty}\rho_{xx}(R,0)=\frac{\xi}{4}\,\frac{2^{1/2}\gamma^{1/4}}{(1+\gamma)^{1/2}}\,(1-h^2)^{1/8}\lim_{N\to\infty}S_{1,0}(1-A'), \tag{4.18a}$$

where

$$\lim_{N\to\infty}A'=\lim_{N\to\infty}(S_{1,0})^{-1}\left(\frac{1}{2\pi i}\oint dz\,z^{-R}[(1-\lambda_1^{-1}z)(1-\lambda_2^{-1}z)]^{-1/2}\right.$$

$$\left.\times\frac{1}{2\pi i}\oint dz'\,\frac{z'^{-R-1}}{z'z-1+\epsilon}\,[(1-\lambda_1^{-1}z')(1-\lambda_2^{-1}z')]^{1/2}\right), \tag{4.18b}$$

and $S_{1,0}$ is given by (4.8b). To first order for large R, $A'\sim A$.

B. $h>1$, $|\lambda_1|>1$, and $|\lambda_2^{-1}|>1$

We define two ratios

$$s_1^2=\det\Xi/\det\Omega_1 \tag{4.19a}$$

and

$$s_2^2=\det\Omega_2/\det\Omega_1, \tag{4.19b}$$

where

$$\Omega_1=\begin{pmatrix} \underline{0}\,| & |\,\underline{S} & \underline{\Gamma}^1 & \underline{\Gamma}^2 & \underline{\Delta}^1 & \underline{\Delta}^2 \\ -\bar{S}^T\,| & |\,\bar{0} & -\bar{E}^1 & -\bar{E}^2 & -\bar{K}^1 & -\bar{K}^2 \\ -\Gamma^{1T}\,| & |\,E^{1T} & 0 & 0 & -S_{1,0} & 0 \\ -\Gamma^{2T}\,| & |\,E^{2T} & 0 & 0 & 0 & -S_{1,0} \\ -\Delta^{1T}\,| & |\,K^{1T} & S_{1,0} & 0 & 0 & 0 \\ -\Delta^{2T}\,| & |\,K^{2T} & 0 & S_{1,0} & 0 & 0 \end{pmatrix} \tag{4.19c}$$

and

$$\Omega_2 = \begin{pmatrix} \underline{0} & \big| \underline{S} \\ -\bar{S}^T & \big| \bar{0} \end{pmatrix} , \quad (4.19d)$$

with the horizontal (vertical) lines indicating added rows (columns). By examining Ω_1^{-1} in a way similar to the treatment of Ξ^{-1} for $h < 1$, we can show that $s_1^2 = 0$. Furthermore, from $\det\Omega_2$ and s_2^2 we find that $\det\Omega_1 \neq 0$. Therefore, we have the exact result

$$\lim_{N\to\infty} \rho_{xz}(R, t) = 0 \quad (4.20)$$

for $h > 1$. (This is in agreement with our symmetry considerations.)

Using the same analytic technique as for $\rho_{xz}(R, t)$, one can show for all $h \geq 0$, $h \neq 1$,

$$\lim_{N\to\infty} \rho_{yz}(R, t) = 0 . \quad (4.21)$$

Again this is exact. (It also follows from the symmetry condition (2.5c) with a statement of continuity in h_x.)

V. DISCUSSION

The large R and t behaviors of the correlation functions are consistent with the dependence MBA found for ρ_{xx} and ρ_{yy}; namely, for $R \to \infty$ the correlation functions fall off exponentially in R for $h \neq 1$ and for $t \to \infty$ as $t^{-1/2}$ for $h > 1$ and t^{-1} for $h < 1$. The difference in the t dependence is caused by a variation in the nature of the states coupling into the dynamics. For $h > 1$ and zero temperature single spin waves are sufficient to describe the system and imply a $t^{-1/2}$ behavior. For $h < 1$ the complete set of states for the first excited states do not consist of single spin waves but consist rather of two spin waves, rendering a $t^{-1/2}$ dependence invalid.

We can explicitly show the difference in character of the first excited states by not changing the boundary condition on H to a cyclic boundary condition in the c space, but, instead, diagonalizing H exactly. This is accomplished by writing (3.2) as

$$H = H^+P^+ + H^-P^- , \quad (5.1a)$$

where

$$H^{\pm} = \frac{1}{2}\left(\sum_1^{N-1} (c_j^\dagger c_{j+1} + c_{j+1}^\dagger c_j + \gamma c_j^\dagger c_{j+1}^\dagger + \gamma c_{j+1} c_j) - 2h\sum_1^N (c_j^\dagger c_j - \tfrac{1}{2}) \mp (c_N^\dagger c_1 + c_1^\dagger c_N + \gamma c_N^\dagger c_1^\dagger + \gamma c_1 c_N)\right) \quad (5.1b)$$

and

$$P^{\pm} = \frac{1}{2}\left[1 \pm \exp\left(i\pi \sum_1^N c_j^\dagger c_j\right)\right] . \quad (5.1c)$$

The eigenstates of H consist of any even number (including 0) of c excitations of H^+ and the odd excitations of H^-. Therefore, one can diagonalize H^+ and H^- separately and select those states of each which are eigenstates of H. The diagonalization of $H^{\pm}$ is performed as indicated earlier; i.e., a Fourier transformation is made with a subsequent Bogoliubov transformation. (For more details, see Ref. 6.)

One finds that

$$H^+ = -\tfrac{1}{2}\textstyle\sum_{\phi^+} \Lambda(\phi^+) + \sum_{\phi^+} \Lambda(\phi^+)\, \eta_{\phi^+}^{(+)\dagger} \eta_{\phi^+}^{(+)} \quad (5.2a)$$

and

$$H^- = -\tfrac{1}{2}\textstyle\sum_{\phi^-} \Lambda(\phi^-) + \sum_{\phi^-} \Lambda(\phi^-)\eta_{\phi^-}^{(-)\dagger} \eta_{\phi^-}^{(-)} , \quad (5.2b)$$

where we sum over $\phi^+ = \pm\pi(2n+1)/N$, with $n = 0, 1, \ldots, N/2 - 1$ and $\phi^- = 0, \pm 2\pi n/N, \pi$, with $n = 1, \ldots, N/2 - 1$. $\Lambda(\phi) = [(\cos\phi - h)^2 + \gamma^2 \sin^2\phi]^{1/2}$ for all $\phi \neq 0$ and $\Lambda(0) = h - 1$.

If we shift the energy by adding $\frac{1}{2}\sum_{\phi^{\pm}}\Lambda(\phi^{\pm})$ to $H^{\pm}$, to order e^{-N} we obtain

$$H^+ = \textstyle\sum_{\phi^+} \Lambda(\phi^+)\eta_{\phi^+}^{(+)\dagger} \eta_{\phi^+}^{(+)} , \quad (5.3)$$

and for $h > 1$

$$H^- = \textstyle\sum_{\phi^-} \Lambda(\phi^-)\eta_{\phi^-}^{(-)\dagger} \eta_{\phi^-}^{(-)} , \quad (5.4)$$

and for $h < 1$

$$H^- = 1 - h + \textstyle\sum_{\phi^-} \Lambda(\phi^-)\, \eta_{\phi^-}^{(-)\dagger} \eta_{\phi^-}^{(-)} . \quad (5.5)$$

Since the Fourier and Bogoliubov transformations which we have performed[6] are such that

$$\exp\left(i\pi \sum_1^N c_i^\dagger c_i\right) = \exp\left(i\pi \sum_{\phi^{\pm}} \eta_{\phi^{\pm}}^{(\pm)\dagger} \eta_{\phi^{\pm}}^{(\pm)}\right) , \quad (5.6)$$

the eigenstates of H consist of the even η excitations of H^+ from $|0_+\rangle$ and the odd η excitations of H^- from $|0_-\rangle$. $|0_+\rangle$ and $|0_-\rangle$ are defined by $\eta_{\phi^+}^{(+)}|0_+\rangle = 0$, all ϕ^+, and $\eta_{\phi^-}^{(-)}|0_-\rangle = 0$, all ϕ^-.

Because $\Lambda(\phi)$ for $h > 1$ is continuous at $\phi = 0$, the H^+ and H^- have easily understood spectra (for $h > 1$). For both H^+ and H^- the ground states are the same as the vacuum states $|0_{\pm}\rangle$ and the excitation spectra lend themselves to an interpretation of particle excitations. We can extract the spectrum of H and find that it contains a nondegenerate ground state with energy zero and eigenstate $|0_+\rangle$. The first excited states of H are the single-particle states $\eta_{\phi^-}^{(-)\dagger}|0_-\rangle$ with energies $\Lambda(\phi^-)$ and possess an interpretation as single spin waves.

For $h < 1$ the spectrum of H^+ still retains its simplicity. However, H^- has significant modifications in its spectrum. $\Lambda(\phi)$ is not continuous at $\phi = 0$ and is, in fact, negative causing the ground state and vacuum state $|0_-\rangle$ of H^- to be two different states. In particular, the ground state of H^- is $\eta_0^{(-)\dagger}|0_-\rangle$ and is nondegenerate with energy equal to zero. Since this state is an odd η excitation, it is in the spectrum of H, thereby leading to a doubly degenerate (to order e^{-N}) ground state for H. One can proceed to discuss the spectrum of H^- in this representation, but one is misled by so doing. The misconceptions that arise are caused by one's desire to label states $\eta_{\phi^-}^{(-)\dagger}|0_-\rangle$, $\phi^-\neq 0$, as single-particle states and, correspondingly, single spin-wave states. However, they are not such states because $\Lambda(0)<0$. It is better to transform $\xi_{\phi^-}=\eta_{\phi^-}^{(-)}$ for $\phi^-\neq 0$ and $\xi_0^\dagger=\eta_0^{(-)}$. Then for $h<1$

$$H^- = |\Lambda(0)|\,\xi_0^\dagger\xi_0+\sum_{\phi^-\neq 0}\Lambda(\phi^-)\xi_{\phi^-}^\dagger\xi_{\phi^-}\,. \tag{5.7}$$

Because of the change of basis, the even ξ excitations of H^- above the new vacuum $|0_-'\rangle$ are eigenstates of H; i.e., because

$$\exp\left(i\pi\sum_{\phi^-}\eta_{\phi^-}^{(-)\dagger}\eta_{\phi^-}^{(-)}\right)=-\exp\left(i\pi\sum_{\phi^-}\xi_{\phi^-}^\dagger\xi_{\phi^-}\right)\,, \tag{5.8}$$

evenness and oddness have switched. $|0_-'\rangle$ is defined by $\xi_{\phi^-}|0_-'\rangle=0$, all ϕ^-. It is now easily seen that the ground state of H is doubly degenerate with eigenstates $|0_+\rangle$ and $|0_-'\rangle$. The first excited states of H consist of the two particle $\eta^{(+)}$ excitations of H^+ and the two-particle ξ excitations of H^-. These can be interpreted as two spin-wave states.

Therefore, for $h>1$ the ground state of H is nondegenerate with energy zero and is the ground state $|0_+\rangle$ of H^+. The first excited states $\eta_{\phi^-}^{(-)\dagger}|0_-\rangle$ (N single-particle states) come from H^- as given by (5.4) and are single spin-wave states with energy equal to $\Lambda(\phi^-)$.

For $h<1$ the ground state of H is doubly degenerate and consists of the ground states, $|0_+\rangle$ and $|0_-'\rangle$, of H^+ and H^-, respectively. The first excited states are the two-particle states, $\eta_{\phi_1}^{(+)\dagger}\eta_{\phi_2}^{(+)\dagger}|0_+\rangle$ and $\xi_{\phi_1}^\dagger\xi_{\phi_2}^\dagger|0_-'\rangle$, of H^+ and H^- as given by (5.3) and (5.7), respectively. There are N^2-N such states, and they correspond to two spin-wave states.

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Circle Theorem for the Ice-Rule Ferroelectric Models*

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We show that the circle theorem on the distribution of zeros of the partition function breaks down for the ferroelectric potassium dihydrogen phosphate (KDP) model if the field lies outside the first quadrant. We also use a recent result by Suzuki and Fisher to establish the circle theorem for the antiferroelectric F model with a staggered electric field. Numerical results on the distribution of zeros for a 4×4 lattice are given.

INTRODUCTION

A central problem in the theory of phase transitions has been the investigation of the distribution of zeros of the partition function.[1] For the Ising ferromagnet in a magnetic field, Lee and Yang[1] showed that all zeros of the partition function lie on the unit circle, a result known as the "circle theorem." This circle theorem has recently been extended to a number of other models.[2] One particular model which has been discussed is the ice-rule ferroelectric model of hydrogen-bonded crystals.[3] For the ferroelectric potassium dihydrogen phosphate (KDP) model Suzuki and Fisher[2] (SF) showed that all zeroes of the partition function with an electric field in the *first quadrant* lie on the unit circle