Decay of Order in Classical Many-Body Systems. II. Ising Model at High Temperatures*

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We employ the transfer-matrix formalism expounded in Paper I to study the decay of pair correlation functions at high temperatures in the d-dimensional Ising model in an arbitrary magnetic field H. A general correlation function decays according to

$$\langle \delta L(\vec{0})\delta Q(\vec{R})\rangle \approx R^{(d-1)/2}\ e^{-\kappa R}(A_0+A_1R^{-1}+\cdots)+R^{-x}e^{-\kappa' R}(B_0+B_1R^{-1}+\cdots)+\cdots$$

as $R\to\infty$. For sufficiently small H and high temperature T, the exponent x is equal to the dimension of the lattice and $\kappa'=2\kappa$. The coefficients A_n and B_n factor as $A_n(Q)A_n(L)$ and $B_n(Q)B_n(L)$, respectively. If $\vec{Q}$ is an operator involving an *odd* number of closely spaced spins, $A_n(Q)$ tends to a finite limit and $B_n(Q)$ tends to zero as H tends to zero. In contrast, if $\vec{Q}$ involves an *even* number of closely spaced spins, $A_n(Q)$ tends to zero and $B_n(Q)$ to a finite limit as H tends to zero. Thus, for finite H an *arbitrary* pair correlation function verifies the Ornstein-Zernike (OZ) prediction; whereas in the zero field, (i) if *both* $\vec{Q}$ and $\vec{L}$ are products of odd numbers of spin operators, $G_{LQ}(\vec{R})$ will verify the OZ prediction in zero field; (ii) if both $\vec{L}$ and $\vec{Q}$ involve even numbers of spins, $G_{LQ}(\vec{R})$ fails to verify the OZ prediction in zero field; and (iii) if $\vec{L}$ involves an odd number of spins while $\vec{Q}$ involves an even number of spins, $G_{LQ}(\vec{R})$ is identically zero in zero field for all $\vec{R}$. The failure of the zero-field Ising model to completely verify the OZ prediction at high temperatures is due to the symmetry of this model about the $H=0$ line.

I. INTRODUCTION

In this work the formalism expounded in Paper I of this series[1(a)] is used to study the decay of pair correlation functions in the d-dimensional Ising model in an arbitrary field H at high temperatures. A sketch of the approach and a statement of the principal results have been previously published.[1(b)] Definitions and formulas developed in I are used throughout—occasionally without explicit reference.

The correlation functions considered are those between two widely separated groups of localized spins; especially those between two widely separated spins, henceforth referred to as spin correlation functions, and those between pairs of nearest-neighbor spins in widely separated layers referred to as energy-density correlations. Both of these latter types are considered in arbitrary magnetic field.

These correlation functions are important for several reasons. First of all, the initial susceptibility of a ferromagnet and the compressibility of a liquid-vapor system are essentially given by the integral of the pair correlation function over the whole system.[2] Secondly, the specific heat is given by the integral of the energy-density correlation function over the system.[2] In addition, the Fourier transform of the pair correlation function determines the cross section for elastic scattering of radiation in the first Born approximation.[3]

However, almost as important as these physical considerations are the constraints the form of the decay of correlations away from the critical point puts on the so-called "scaling forms" for the decay of correlations in the critical region.[4] For a thorough discussion of these scaling forms, refer to Fisher and Burford.[5] We briefly sketch their scaling form for the spin correlation function and the relevance of our work to such forms.

Based on exactly known two-dimensional correlation functions and on numerical studies in three dimensions, Fisher and Burford[5] proposed the following form for the Ising spin correlation function:

$$G_s(\vec{R})\equiv\langle\delta S^z(\vec{0})\delta S^z(\vec{R})\rangle = D(\kappa R)e^{-\kappa R}/R^{(d-2+\eta)}, \quad (1.1)$$

where $D(x)\approx x^{(d-3+2\eta)/2}$ as x tends to infinity, and $D(x)\approx 1+o(1)$ as x tends to zero. Thus, the correlations *within* the critical region are predicted to behave like

$$G_s(R)\sim e^{-\kappa R}/R^{d-2+\eta}\ \text{ as } \kappa R\to 0\,, \quad (1.2)$$

while outside the critical region spin correlations are expected to decay as

$$G_s(R)\sim \kappa^{(d-3+2\eta)/2}(e^{-\kappa R}/R^{(d-1)/2})\ \text{ as } \kappa R\to\infty\,. \quad (1.3)$$

This form was chosen in order to reproduce the Ornstein-Zernike (OK) form[1] for the decay of correlations outside the critical region and to reproduce the results found for the decay of correlation in the critical region in the two- and three-dimensional Ising model [Eq. (1.2)], with $\eta=\frac{1}{4}(d=2)$, and

$\eta \approx 0.06 (d=3)$.[5] One aspect of our work is to answer the general question of when to expect OZ behavior outside the critical region.

For any $T \neq T_c$, we may integrate (1.1) to find χ_T, the initial susceptibility. Thus, we have

$$\chi_T \approx \chi_0 \kappa^{-(2-\eta)}, \quad T \to T_c^+ \tag{1.4}$$

where χ_0 depends only weakly on temperature. The critical exponent ν is defined by the relation $\kappa \sim (T - T_c)^{\nu}$ as T tends to T_c from above, and the exponent γ is defined by $\chi_T \sim (T - T_c)^{-\gamma}$ as T tends to T_c from above. Thus, from (1.4), we expect that

$$(2-\eta)\nu = \gamma . \tag{1.5}$$

Relationships such as (1.5) are known as scaling relations.[6-10] Most of these scaling relations among the critical exponents have been proven as inequalities.[11]

A previously unresolved question in scaling theory is when the OZ form (1.3) outside the critical region can be expected. The exact results[12,13] for the zero-field two-dimensional nearest-neighbor Ising model at low temperatures demonstrate that (1.3) does *not* hold in this case. However, for the spin pair correlation function at high temperatures in this system,[12,14,15] (1.3) is found to hold. Thus, a single scaling form such as (1.1) cannot correctly describe the decay of correlation over the whole thermodynamic surface. Further, the decay of energy-density correlation functions in the zero-field two-dimensional Ising model at high temperatures is known to be non-Ornstein-Zernike-like.[13] Thus, the scaling forms for the spin and the energy-density correlation functions must differ in their asymptotic behavior—as indeed found by Hecht.[13]

We cannot say anything rigorously about scaling since our results are proven only asymptotically as $T^{\pm 1} \to 0$. However, there are quite strong reasons to believe that the correlation functions have a single asymptotic form everywhere outside the critical region.[16] Thus, we expect to be able to state generally when to expect OZ behavior outside the critical region. A map of the critical region and the region in which our perturbative results are assuredly valid in the R-ξ plane, is given in Fig. 1, with the critical region cross hatched and the region of known validity of our work diagonally barred. Since we expect our functional forms for the decay of correlations to remain valid except in the critical region of the R-ξ plane (even though we have explicitly assumed $\kappa R \gg 1$, $R \gg 1$, in deriving them), we maintain that our results determine $D(x)$ as $x \to \infty$ in the Fisher-Burford scaling form [Eq. (1.1)].

The information known about the decay of energy-density correlation functions is much sketchier than that for the spin correlation function. The major previous results are the exact *zero-field* calculations by Stephenson[13] and by Hecht[13] in *two* dimensions. The latter author found that the energy-density correlation function $G_E(\vec{R})$ is given near T_c by

$$G_E(\vec{R}) \equiv \langle \delta E(\vec{0})\, \delta E(\vec{R}) \rangle = (2J/\pi)^2\, 2\kappa_E^2(K) \times [\mathcal{K}_1^2(2\kappa_E R) - \mathcal{K}_0^2(2\kappa_E R)] , \tag{1.6}$$

where, as above, $K = \beta J$, $\kappa_E \approx 2K[(K/K_c)/-1]$, and $\mathcal{K}_n(x)$ is the modified Bessel function of the second kind, of order n.[13] This may easily be asymptotically analyzed to find that

$$G_E(\vec{R}) \approx (2J^2/\pi)\, (e^{-\kappa_E R}/R^2), \quad R \gg 1, \quad \kappa_E \ll 1, \tag{1.7a}$$

$$G_E(\vec{R}) \approx (4J^2/\pi)\, (1/R^2), \quad R \ll 1, \quad \kappa_E \ll 1 . \tag{1.7b}$$

Thus, if we write the zero-field correlation function as

$$G_E(\vec{R}) = D_0(\kappa_E R)\, e^{-\kappa_E R}/R^{d-2+\eta_\epsilon} , \tag{1.8}$$

we expect, both as x and $1/x$ tend to zero, that

$$D_0 \sim x^{\eta_\epsilon - 2} . \tag{1.9}$$

This result is significantly different from that found above for the spin correlation function. However, it has been conjectured[17] that for finite magnetic field, the spin and the energy-density correlation functions will be of the same form and that only for zero field above T_c are they significantly different.

The work reported herein (and summarized by Camp and Fisher[1(b)]) yields a qualitative understanding of this behavior. As we noted above, given the finiteness of appropriate matrix elements, the decay of correlations is determined by the single-particle eigenstates of the transfer matrix.[1] The corrections to this leading term are then provided by the two-particle band. Below we show that this implies the following form for a general correlation function at high temperatures[1(b)]:

$$G(\vec{R}) \approx \frac{e^{-\kappa R}}{R^{(d-1)/2}} \left(A_0 + \frac{A_1}{R} + \cdots \right) + \frac{e^{-\kappa' R}}{R^{x}} \left(B_0 + \frac{B_1}{R} + \cdots \right) \text{ as } R \to \infty , \tag{1.10}$$

where, for sufficiently small fields and high temperatures, $x = d$ and κ' is given by 2κ. The coefficients A_n are determined by matrix elements of the correlated operators between the largest eigenvector and the states of the single-particle band, while the B_n are determined by matrix elements between the largest eigenvector and the two-particle states. For the spin correlation function the sequence $\{A_n\}$ approaches a nonzero limit as the field h tends to zero while $\{B_n\}$ tends to zero. However,

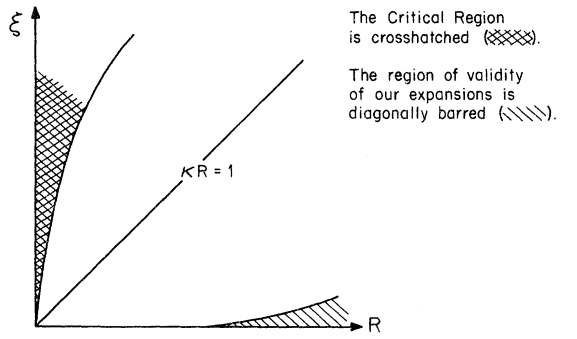

FIG. 1. $R-\xi$ plane. Although our expansion is most accurate for $\kappa R \gg 1$, we expect our functional forms to hold everywhere outside the critical region, $\kappa R \ll 1$.

for the energy-density correlation function, A_n may be expanded as $A_{n,2}h^2+A_{n,4}h^4+\cdots$, while $B_n=B_{n,0}+h^2B_{n,2}+\cdots$. Thus in zero field, the decay of energy-density correlations is qualitatively different from that in a small, but finite, field. In the former case, the ultimate decay form is determined by the two-particle band and in the latter case by the single-particle band. This statement is shown to be correct to *all* orders in the perturbation expansion—and thus may be generally correct for T above T_c.

If one assumes complete scaling for the correlation functions,[18] a general correlation function $G(\vec{R})$ is written

$$G(\vec{R}) = R^{-d+2-\eta_x}\,\tilde{G}(tR^{\phi_x},\, hR^{d-\Psi_x}) , \qquad (1.11)$$

where x labels the type of correlation function,

$$\gamma\phi_x = (2-\eta_x),$$

and

$$\Psi_x = \tfrac{1}{2}(d-2+\eta_x) ,$$

where γ is the critical index for the susceptibility. The variable t is a reduced temperature $t=T/T_c-1$. Assuming this work to be relevant to the scaling forms, the following results are evident. For the spin correlation function $\tilde{G}_s(x,y)$ approaches a single functional form in the variables κ and R as x tends to infinity for *any* value of y. This functional form is just $(\kappa R)^{(d-3+\eta_x)/2}\,e^{-\kappa R}$, which reproduces the OZ result as $x=(\kappa R)^{1/\nu}$ tends to infinity. On the other hand, $\tilde{G}_\epsilon(x,y)$ for the energy-density correlation function approaches a different limit as x tends to infinity, depending upon whether y remains zero or finite, or also tends to infinity. If y remains zero or finite as x tends to infinity, $\tilde{G}_\epsilon(x,y)$ behaves as $(\kappa R)^{\eta_\epsilon-2}\,e^{-\kappa R}$. But, if y also tends to infinity as x tends to infinity, we find $\tilde{G}_\epsilon(x,y)$ behaving as $(\kappa R)^{d-3+\eta_\epsilon/2}\,e^{-\kappa R}$. This indicates a nontrivial difference between the complete scaling forms for $G_s(\vec{R})$ and $G_\epsilon(\vec{R})$.

A less tenuous result of our work is the following. One is led to propose a restricted scaling form in the variable $\kappa(h,\,T)R$ of the form

$$G_\epsilon(\vec{R}) = e^{-\kappa R}D(h,\,\kappa R)/R^{d-2+\eta_\epsilon} , \qquad (1.12)$$

with, for small h,

$$D(h,\,x) = D_0(x)+h^2D_1(x)+O(h^4) . \qquad (1.13)$$

The functions $D_0(x)$ and $D_1(x)$ obey

$$D_0(x)\sim x^{\eta_\epsilon-2}\,e^{-x} \text{ as } x^{\pm1}\to\infty \qquad (1.14a)$$

and

$$D_1(x)\sim x^{(d-3+2\eta_\epsilon)/2} \text{ as } x\to\infty . \qquad (1.14b)$$

The behavior described in (1.14a) as $x\to\infty$ is deduced from our results; and that as $x\to 0$ is generalized from Hecht's[13] two-dimensional results. The behavior of $D_1(x)$ for $x\to\infty$ is also deduced from the work below. Note that $D_0(x)$ and $D_1(x)$ depend upon h only through κR. If we assume (1.13) holds for strictly finite h, then κR is never zero in $D_1(\kappa R)$ as long as h is nonzero.[19] In any case we cannot comment upon the behavior of $D_1(x)$ as $x\to 0$ because of our restriction to $\kappa R\gg 1$, and $R\gg 1$.

The energy-density correlation functions satisfy the specific-heat sum rule mentioned above; that is, the integral of $G_\epsilon(\vec{R})$ over the entire system yields the specific heat. In zero field the specific heat diverges as $C_{H=0}\sim(T/T_c-1)^{-\alpha}$, $T\to T_c^+$; so, from (1.12) and (1.14a) we have $(2-\eta_\epsilon)\nu=\alpha$. This may be taken as defining η_ϵ and hence as constraining $D_1(x)$ as $x\to\infty$ and $D_0(x)$ as $x\to 0$ or ∞.

The outline of this work is as follows. In Secs. II and III we obtain the Ising transfer matrix in a form suitable for high-temperature perturbation theory and examine the eigenvalue spectrum via perturbation theory.[1(b)] In Secs. IV and V we obtain the decay of spin and energy-density correlation functions, respectively. The angular dependence of κ, the inverse correlation length, is also produced in Sec. IV. Section VI is a summary of our results.

II. HAMILTONIAN AND TRANSFER MATRIX OF THE SYSTEM

The system treated herein is the spin-half ($s=\frac{1}{2}$) Ising model. In this model one associates a two-valued variable $S(\vec{r})=\pm 1$ with each lattice site $\vec{r}$. In a model for magnetism one may associate $S(\vec{r})$ with the z component of a spin angular momentum. Then the $S=+1$ state corresponds to a spin aligned upward along the positive z direction, while $S=-1$ corresponds to a spin aligned downward along the negative z direction. (Hence, we shall speak of spin-up and spin-down states when S equals $+1$ and -1, respectively.) Alternately, one may think of the model as a "lattice gas" obtained by associating an occupation number $t(\vec{r})=\frac{1}{2}[1-S(\vec{r})]$ with each site. A site is unoccupied if $t=0$, i.e., if $S=+1$.

Notice that this model automatically contains a "hard core" because each site is, at most, singly occupied.

Having associated a kinematical variable with each lattice site, one specifies the interactions between sites by means of these variables. We again take $\hat{z}$ to be the layering direction of a d-dimensional system and the interactions to be such that only spins in nearest-neighbor $(d-1)$-dimensional hyperplanes interact. Then the layers may be taken to be these hyperplanes. Every lattice vector $\vec{R}$ is of the form

$$\vec{R} = \vec{r}_\perp + \hat{z} r_\parallel \ . \tag{2.1}$$

The notation is self-explanatory—$r_\parallel$ labels the layer (the component of $\vec{R}$ parallel to $\hat{z}$), and $\vec{r}_\perp$ is an arbitrary vector lying within a given layer (perpendicular to the layering axis $\hat{z}$). Throughout this work the lattice spacing is assumed to be unity. Although it would be useful to allow second-neighbor interactions between layers—interactions connecting $(\vec{r}_\perp, l\hat{z})$ and $[\vec{r}_\perp + \vec{\delta}, (l+1)\hat{z}]$ with $\vec{\delta}$ a nearest-neighbor layer vector, we shall not do so since allowing such interactions makes the detailed calculations considerably more involved. However, we shall treat further-neighbor interactions strictly within a layer.

Thus, the Hamiltonian is written

$$-\beta\mathcal{H}_L = \sum_{\vec{x}} \sum_l [K_\parallel S(\vec{x}, l) S(\vec{x}, l+1) + \tfrac{1}{2} K_\perp \sum_{\vec{r}} \varphi(\vec{r}) S(\vec{x}, l) S(\vec{x}+\vec{r}, l) + h S(\vec{x}, l)] \ . \tag{2.2}$$

In (2.2), $\beta = (k_B T)^{-1}$, $K_\parallel = \beta J_\parallel$, $K_\perp = \beta J_\perp$, and $h = \beta g H$, where T is the temperature, k_B is Boltzmann's constant, $J_\parallel$ and $J_\perp$ are exchange energies, g is the Landé factor, and H is the magnetic field. $\varphi(\vec{r})$ is a dimensionless intralayer "interaction shape function." The vectors $\vec{x}$ and $\vec{r}$ lie entirely within a layer, and l is the layer index. The range of summation of l depends upon the boundary conditions in the z direction, while the range of summation of $\vec{x}$ and $\vec{r}$ depend upon the boundary conditions imposed upon the layers proper.

With this definition of the Hamiltonian, one easily writes down the transfer matrix $\underline{K}$ via its 4^N-matrix elements between states of the lth and $(l+1)$th layers[1]:

$$\underline{K}(\alpha_l, \alpha_{l+1}) = \exp\{\sum_{\vec{x}} [K_\parallel S(\vec{x}, l) S(\vec{x}, l+1) + \tfrac{1}{2} K_\perp \sum_{\vec{r}} \varphi(\vec{r}) S(\vec{x}, l) S(\vec{x}+\vec{r}, l) + h S(\vec{x}, l+1)]\} \ . \tag{2.3}$$

It is shown below that $\underline{K}$ has a natural division as the product of three matrices:

$$\underline{K} = \underline{K}_a(K_\parallel) \cdot \underline{K}_b(K_\perp) \cdot \underline{K}_c(h) \ , \tag{2.4}$$

where the latter two matrices are diagonal (and hence commute) while the first is nondiagonal. A particularly simple expression for all three matrices may be found in terms of Pauli spin operators $\underline{\sigma}^x$, $\underline{\sigma}^y$, $\underline{\sigma}^z$, and $\underline{I}$. In the $\underline{\sigma}^z$ representation, these are

$$\underline{\sigma}^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \underline{\sigma}^y = i \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}, \quad \underline{\sigma}^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \underline{I} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \tag{2.5}$$

(Notice that one may expand *any* 2×2 matrix in terms of these four matrices.)

For simplicity we initially formulate the problem for the case of a double chain of spins. All the essential features of the general case are included, while the matrix algebra is simple enough to be transparent. The transfer matrix for the double chain depicted in Fig. 2 is

$$\underline{K}(1, 2) = \exp\{K_\parallel (S_{11} S_{21} + S_{12} S_{22})\} \exp(K_\perp S_{21} S_{22}) \times \exp[h(S_{21} + S_{22})] \ . \tag{2.6}$$

This transfer matrix has the form $A(i,j) = a(i,j) \times b(j) c(j)$ and may easily be written

$$A(i,j) = \sum_k \sum_l a(i,k) \{b(k) \delta(k,l)\} \{c(l) \delta(l,j)\} \ , \tag{2.7}$$

where $\delta(i,j)$ is the Kronecker δ, equal to 1 if i equals j, and 0 otherwise; hence, $\underline{A}$ is clearly seen to be the matrix product $\underline{a}\,\underline{b}\,\underline{c}$ with $\underline{b}$ and $\underline{c}$ diagonal. Thus, $\underline{K}$ is written

$$\underline{K} = \underline{K}_a \cdot \underline{K}_b \cdot \underline{K}_c \ , \tag{2.8}$$

with

$$\underline{K}_a(\vec{1}, \vec{2}) = e^{K_\parallel (S_{11} S_{21} + S_{12} S_{22})} \ , \tag{2.9a}$$

$$\underline{K}_b(\vec{1}, \vec{2}) = \delta(S_{11}, S_{21}) \delta(S_{12}, S_{22}) e^{K_\perp \cdot S_{21} S_{22}} \ , \tag{2.9b}$$

$$\underline{K}_c(\vec{1}, \vec{2}) = \delta(S_{11}, S_{21}) \delta(S_{12} S_{22}) e^{h(S_{21} + S_{22})} \ . \tag{2.9c}$$

The latter two matrices are explicitly diagonal; in fact

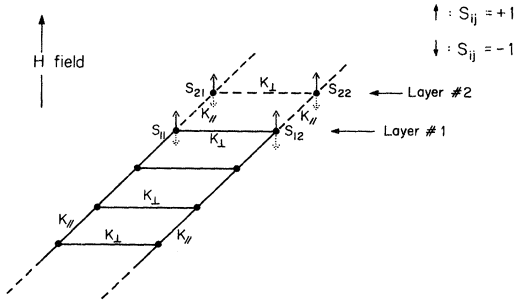

FIG. 2. Double Ising chain in a magnetic field.

$$\underline{K}_a = \left[\begin{array}{cc:cc} e^{2K_\parallel} & 1 & 1 & e^{-2K_\parallel} \\ 1 & e^{2K_\parallel} & e^{-2K_\parallel} & 1 \\ \hdashline 1 & e^{-2K_\parallel} & e^{2K_\parallel} & 1 \\ e^{-2K_\parallel} & 1 & 1 & e^{2K_\parallel} \end{array}\right] ,$$

$$\underline{K}_b = \left[\begin{array}{cc:cc} e^{K_\perp} & 0 & & \\ 0 & e^{-K_\perp} & & \\ \hdashline & & e^{K_\perp} & 0 \\ & & 0 & e^{-K_\perp} \end{array}\right] , \qquad (2.10)$$

$$\underline{K}_c = \left[\begin{array}{cc:cc} e^{2h} & 0 & & \\ 0 & 1 & & \\ \hdashline & & 1 & 0 \\ & & 0 & e^{-2h} \end{array}\right] .$$

It is convenient to use the notion of the direct product of matrices.[20] For example, with definition (2.5), if $\underline{\sigma}^x(1)\underline{\sigma}^z(2)$ is the direct product of $\underline{\sigma}^x$ in the first space and $\underline{\sigma}^z$ in the second, then one may write

$$\underline{\sigma}^x(1)\underline{\sigma}^z(2) = \left[\begin{array}{cc:cc} & & 1 & 0 \\ & & 0 & -1 \\ \hdashline 1 & 0 & & \\ 0 & -1 & & \end{array}\right] , \qquad (2.11)$$

Further in direct products, such as $\underline{I}(1)\underline{\sigma}^\mu(2)$, involving the identity matrix, we suppress the identity matrix and simply write $\underline{\sigma}^\mu(2)$. Using the Van der Waerden identities[21] and introducing the variable $u_\parallel$ via

$$\tanh(u_\parallel) = e^{-2K_\parallel} , \qquad (2.12)$$

one has

$$\underline{K}_a = 2\sinh(2K_\parallel)\exp\{u_\parallel[\underline{\sigma}^x(1)+\underline{\sigma}^x(2)]\} ,$$
$$\underline{K}_b = \exp[K_\perp\underline{\sigma}^z(1)\underline{\sigma}^z(2)] , \quad \underline{K}_c = \exp\{h[\underline{\sigma}^z(1)+\underline{\sigma}^z(2)]\} ; \qquad (2.13)$$

or equivalently, $\underline{K}_1 = \underline{K}_1\underline{K}_2$, with $\underline{K}_1 = \underline{K}_a\underline{K}_c$ and $\underline{K}_2 = \underline{K}_b$. Note that $\underline{K}_1$ allows for interactions along a chain while $\underline{K}_2$ puts in the interaction between chains. Below we see that at high temperatures $\underline{K}_2$ must be treated perturbatively.[1(b)] We thus have included the field dependence in $\underline{K}_1$ rather than (unnecessarily) also treating it perturbatively.

The concept of direct product extends to arbitrary dimensional spaces. Using this concept and simple algebra, we write the general $\underline{K}$ defined in (2.3) as

$$\underline{K} = \{\prod_{\vec{r}}[2\sinh(2K_\parallel)]^{1/2} e^{u_\parallel \underline{\sigma}^x(\vec{r})} e^{h\underline{\sigma}^z(\vec{r})}\} \times \{\exp[\tfrac{1}{2}K_\perp \sum_{\vec{r},\vec{\delta}} \varphi(\vec{\delta})\underline{\sigma}^z(\vec{r})\underline{\sigma}^z(\vec{r}+\vec{\delta})]\} . \qquad (2.14)$$

Writing $\underline{K} = \underline{K}_1\underline{K}_2$, we can either define K_1 as

$$\underline{K}_1 = [2\sinh(2K_\parallel)]^{N/2}\prod_{\vec{r}} e^{u_\parallel \underline{\sigma}^x(\vec{r})} \qquad (2.15)$$

or as

$$\underline{K}_1 = [2\sinh(2K_\parallel)]^{N/2}\prod_{\vec{r}} e^{u_\parallel \underline{\sigma}^x(\vec{r})} e^{h\underline{\sigma}^z(\vec{r})} , \qquad (2.16)$$

where N is the number of sites in a layer, or equivalently the number of chains. In the first case, the magnetic terms are kept in $\underline{K}_2$, whereas in the second case all the magnetic dependence is in $\underline{K}_1$. In either case we can write $\underline{K}_1$ as the direct product of N independent "chain matrices" $\underline{k}_1(\vec{r})$:

$$\underline{K}_1 = \prod_{\vec{r}} \underline{k}_1(\vec{r}) . \qquad (2.17)$$

This matrix is then the full transfer matrix for uncoupled chains, and we may diagonalize each $\underline{k}_1(\vec{r})$ for arbitrary h. Then the limit h tending to zero yields $\underline{k}_1(r)$ appropriate to the choice (2.15). We then have

$$\underline{k}_1 = [2\sinh(2K_\parallel)]^{1/2} e^{u_\parallel \underline{\sigma}^x} e^{h\underline{\sigma}^z} . \qquad (2.18)$$

Let the eigenvalues of $\underline{k}_1$ be $\mu_\pm = [2\sinh(2K_\parallel)]^{1/2}\nu_\pm$; then the secular equation becomes

$$0 = \nu_+ - \cosh(u_\parallel)\{\cosh(h)+[\sinh^2(h)+\tanh^2(u_\parallel)]^{1/2}\} , \qquad (2.19)$$
$$0 = \nu_- - \cosh(u_\parallel)\{\cosh(h)-[\sinh^2(h)+\tanh^2(u_\parallel)]^{1/2}\} ,$$

when

$$\mu_\pm = e^{K_\parallel}\{\cosh(h)\pm[\sinh^2(h)+e^{-4K_\parallel}]^{1/2}\} . \qquad (2.20)$$

Note that $u_\parallel$ has completely disappeared from the problem. We shall see, however, that at low temperatures where $\underline{K}_2$ becomes our "unperturbed" matrix $u_\parallel$ will remain in the problem as a small expansion parameter. In the high-temperature case, which we now consider, $K_\perp = J_\perp/k_BT$ turns out to be our natural expansion parameter. In the limit that $K_\perp = 0$, then $\underline{K} = \underline{K}_1$ and we think of the intralayer interactions in $\underline{K}_2$ as a perturbation on the spectrum of $\underline{K}_1$. Thus, we write $\underline{K} = \underline{K}_1\underline{K}_2$ in the representation in which $\underline{K}_1$ is diagonal. Let $|0\rangle$ be the larger eigenvector and $|1\rangle$ the smaller eigenvector of $\underline{k}_1$, so that

$$\underline{k}_1|0\rangle = \mu_+|0\rangle , \quad \underline{k}_1|1\rangle = \mu_-|1\rangle . \qquad (2.21)$$

We introduce raising and lowering operators $\underline{\psi}^\dagger$ and $\underline{\psi}$ through

$$\underline{\psi}^\dagger|0\rangle = |1\rangle , \quad \underline{\psi}^\dagger|1\rangle = 0 ,$$
$$\underline{\psi}|1\rangle = |0\rangle , \quad \underline{\psi}|0\rangle = 0 . \qquad (2.22)$$

If $\underline{n} = \underline{\psi}^\dagger\underline{\psi}$, we have

$$\underline{n}|0\rangle = 0, \quad \underline{n}|1\rangle = 1|1\rangle , \tag{2.23}$$

where $\underline{n}$ is a number operator. A simple representation for $\underline{k}_1$ is then

$$\underline{k}_1 = \mu_+ e^{-w_{\parallel}\underline{n}} , \tag{2.24}$$

with $w_{\parallel}$ given by $\mu_- = \mu_+ e^{-w_{\parallel}}$.

In the case $N > 1$, using direct-product notation, we can immediately write $\underline{K}_1$ as

$$\underline{K}_1 = \mu_+^N \exp[-w_{\parallel}\textstyle\sum_{\vec{r}} \underline{n}(\vec{r})] , \tag{2.25}$$

where $\underline{n}(\vec{r}) = \underline{\psi}^\dagger(\vec{r})\underline{\psi}(\vec{r})$. Since they are direct-product operators, the creation and annihilation operators for different chains commute. However, operators involving the same chain satisfy an anti-commutation relation. Hence, we have

$$\begin{aligned} &[\underline{\psi}(\vec{r}), \underline{\psi}^\dagger(\vec{r}')] = \delta(\vec{r}, \vec{r}')\,[1 - 2\underline{n}(\vec{r})] , \\ &[\underline{\psi}(\vec{r}), \underline{\psi}(\vec{r}')] = 0 , \quad [\underline{\psi}(\vec{r}), \underline{\psi}^\dagger(\vec{r})] = 1 . \end{aligned} \tag{2.26}$$

We may think of $\underline{\psi}^\dagger(\vec{r})$ as creating a "particle" on site r. With this analogy, we see that (a) the states of $\underline{K}_1$ are states of given particle number, and (b) at most, one particle may occupy a site. These operators obey Bose-like commutation rules for particles on different sites and Fermi-like rules for particles on the same site. The same rules characterize the spin angular momentum operators $[\underline{\sigma}^{\pm}(\vec{r})]$ and are known as Pauli commutation rules—hence these particles are sometimes referred to as Pauli particles. It is just this hybridization of Fermi and Bose rules which makes spin problems difficult to treat. It is easily seen that Fermi-like or Bose-like rules are unchanged by a Fourier transformation so that if we Fourier transform a particular quadratic form involving Bose or Fermi particles in order to diagonalize it, the structure of the phase space is not changed; that is, the trace operation which is required to obtain the thermodynamics, for instance, is still easily performed. However, for Pauli particles a similar Fourier transformation makes the algebraic structure of the operators very complicated. Thus, the phase space is very complicated, and, even though our quadratic form is diagonal, we are not able to perform the trace operation. The well-known analogy between Pauli and Bose particles with hard cores, on a lattice, is evident from (2.26).[1(b)]

The spectrum of $\underline{K}_1$ is now transparent. The largest eigenvalue is unique and occurs in the state $|\Phi\rangle$ with all chains in their larger eigenvalue. Therefore, $|\Phi\rangle$ is known as the vacuum or zero-particle state. We have

$$\underline{K}_1|\Phi\rangle = \mu_+^N|\Phi\rangle, \quad \Lambda_0 = \mu_+^N . \tag{2.27}$$

The next-largest eigenvalue is $\Lambda_1 = \mu_+^{N-1}\mu_-$ and corresponds to the N single-particle states: $|\vec{r}\rangle = \underline{\psi}^\dagger(\vec{r})|\Phi\rangle$. There are a total of $N+1$ eigenvalues $\{\Lambda_n\}$ with associated degeneracies $\binom{N}{n}$, where n labels the particle number. Consider an n-particle state

$$|\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_n\rangle = \underline{\psi}^\dagger(\vec{r}_1)\underline{\psi}^\dagger(\vec{r}_2)\cdots\underline{\psi}^\dagger(\vec{r}_n)|\Phi\rangle ; \tag{2.28}$$

it is an eigenvector of $\underline{K}_1$ with eigenvalue Λ_n:

$$K_1|\vec{r}_1, \ldots, \vec{r}_n\rangle = \Lambda_n|\vec{r}_1, \ldots, \vec{r}_n\rangle, \quad \Lambda_n = \mu_+^{N-n}\mu_-^n . \tag{2.29}$$

The degeneracy of the n-particle level $g_n = \binom{N}{n}$ arises because there are $N(N-1)\cdots(N-n+1)$ ways of putting n particles into N sites, with at most one particle in a site; and, since the particles are indistinguishable, we need divide by $n!$ for the $n!$ particle interchanges which leave a given configuration unchanged.

In order to express $\underline{K}_2$ in the representation of diagonal $\underline{K}_1$, we need only find $\underline{\sigma}^x(\vec{r})$ in terms of $\underline{I}$, $\underline{n}(r)$, $\underline{\psi}(\vec{r})$, and $\underline{\psi}^\dagger(\vec{r})$. For $h = 0$, or for the case in which all h-dependent terms are in $\underline{K}_2$, the representation of $\underline{\sigma}^x(\vec{r})$ is particularly simple. For then the column vectors of $|0\rangle$ and $|1\rangle$ in the $\underline{\sigma}^x$ representation are

$$\langle\underline{\sigma}^x|0\rangle = 2^{-1/2}\begin{pmatrix}1\\1\end{pmatrix}, \quad \langle\underline{\sigma}^x|1\rangle = 2^{-1/2}\begin{pmatrix}1\\-1\end{pmatrix} , \tag{2.30}$$

from which it follows that

$$\underline{\sigma}^x(\vec{r}) = \underline{\psi}(\vec{r}) + \underline{\psi}^\dagger(\vec{r}) , \tag{2.31}$$

and the transfer matrix becomes

$$\begin{aligned} \underline{K} = \mu_+^N \exp\Big[-w_{\parallel}\sum_{\vec{r}}\underline{n}(\vec{r})\Big] \exp\Big\{\tfrac{1}{2}K_\perp \sum_{\vec{r},\vec{\delta}} \varphi(\vec{\delta})\,[\underline{\psi}(\vec{r}) + \underline{\psi}^\dagger(\vec{r})] \\ \times [\underline{\psi}(\vec{r}+\vec{\delta}) + \underline{\psi}^\dagger(\vec{r}+\vec{\delta})]\Big\} \exp\Big\{h\sum_{\vec{r}}[\psi(\vec{r}) + \underline{\psi}^\dagger(\vec{r})]\Big\} . \end{aligned} \tag{2.32}$$

We reiterate that the disadvantage of (2.32) is that for finite fields and or d greater than two, we are limited to a perturbation-theoretic treatment of $\underline{K}$. If we write

$$\underline{K} = \underline{K}_1 + \underline{K}_1(\underline{K}_2 - \underline{I}) \tag{2.33}$$

at high temperatures ($K_\perp$ being small), we see that $\underline{K}_1(\underline{K}_2 - \underline{I})$ may be treated as a small perturbation upon $\underline{K}_1$. Thus, in using (2.32) at high temperatures, we relegate h (unnecessarily) to a perturbative treatment. On the other hand, if h is nonzero in $\underline{K}_1$, the representation of $\underline{\sigma}^x(\vec{r})$ is more complicated. Now we define the basic single-chain matrix elements which will enter crucially into our subsequent analysis, namely,

$$\begin{aligned} &S_{++} = \langle 0|\underline{\sigma}^x|0\rangle ; \quad S_{+-} = \langle 0|\underline{\sigma}^x|1\rangle , \\ &S_{-+} = \langle 1|\underline{\sigma}^x|0\rangle ; \quad S_{--} = \langle 1|\sigma^x|1\rangle . \end{aligned} \tag{2.34}$$

Then we have

$$\underline{\sigma}^{z}(\vec{r}) = S_{++}\,\underline{I} + (S_{--} - S_{++})\,\underline{n}(\vec{r}) + S_{+-}\underline{\psi}^{\dagger}(\vec{r}) + S_{-+}\underline{\psi}(\vec{r}) \ . \tag{2.35}$$

Using (2.34) for $\underline{\sigma}^{z}(\vec{r})$, we can formally write $\underline{K}$ as

$$\underline{K} = \mu_{+}^{N} \exp\Big[- w_{\parallel} \sum_{\vec{r}} \underline{n}(\vec{r}) \Big] \times \exp\Big[\tfrac{1}{2} K_{\perp} \sum_{\vec{r},\vec{\delta}} \varphi(\vec{\delta})\, \underline{\sigma}^{z}(\vec{r})\underline{\sigma}^{z}(\vec{r}+\vec{\delta})\Big] \ . \tag{2.36}$$

Having (2.32) or (2.36) with (2.35) at hand, we are in a position to remove the degeneracy in the spectrum of $\underline{K}$ and then to calculate via perturbation theory the thermal and microscopic quantities of interest. Since $\underline{K}_1$ and $\underline{K}_2$ do not commute, $\underline{K}_1(\underline{K}_2 - \underline{I})$ is non-Hermitian, even though $\underline{K}_1$ and $\underline{K}_2$ taken separately are Hermitian. Thus, we shall have to use an extension of Rayleigh-Schrödinger perturbation theory[20] to non-Hermitian operators. Since our matrix is positive semidefinite, the eigenvalues will still be real. The essential complication turns out to be only that the left- and right-hand eigenvectors need to be treated separately—$\langle \lambda_t | \rangle^{*} \neq \langle \lambda_t | \rangle$, and that $\langle \Lambda | \underline{K}_1(\underline{K}_2 - \underline{I}) | \Lambda' \rangle \neq \langle \Lambda' | \underline{K}_1(\underline{K}_2 - \underline{I}) | \Lambda \rangle^{*}$ in the determination of higher-order eigenvalues.

III. TRANSFER MATRIX SPECTRUM: ZERO-PARTICLE, SINGLE-PARTICLE, AND TWO-PARTICLE LEVELS

In this section we calculate via degenerate perturbation theory the zero-particle, single-particle, and two-particle eigenvalues and eigenvectors of $\underline{K}$. First, the largest eigenvalue λ_0 is obtained to second order in the coupling constant $K_{\perp}$, while its states $|\lambda_0\rangle$ and $\langle\lambda_0|$ are found to first order in $K_{\perp}$. Then we break the degeneracy of the N single-particle states; they are found to spread out to form a band of levels labeled by a $(d-1)$-dimensional wave vector $\vec{q}$. Again the states are found to first order and the eigenvalues to second order in $K_{\perp}$. These calculations are performed in an arbitrary field and for cyclic boundaries within the layer.

For the two-dimensional case,[5,22] it is straightforward to break the degeneracy of the mth level, $m = 1, 2, \ldots, N-1$. The zeroth-order eigenstates are found to be Slater determinants of m single-particle zeroth-order eigenstates (which are, themselves, running waves). Thus, the particles are found to be Fermi-like. However, in three or more dimensions, in solving for the m-particle eigenvalues and eigenstates, we have essentially to solve the problem of m spin waves for an anisotropic Heisenberg model of dimension $d-1$.[23] In zero magnetic field the problem is somewhat simpler in that we need to solve the (simpler) analogous problem for an X-Y model.[23] The full Heisenberg problem is extremely involved and is characterized by the appearance of bound states of m spins ($m \geq 2$).[23] Thus, consideration of this problem is too ambitious an undertaking to be realistically pursued here. Fortunately, as we see below, it is also largely unnecessary for our purposes. The zero-field case is simpler in that there exists no such bound states in the spectrum. Whereas in zero field the two-particle spectrum is necessary for an understanding of the decay of, for example, energy-density correlation functions, in a finite field the single-particle spectrum suffices for all correlations. We are able to solve the two-particle zero-field problem, which we treat in Sec. IV, in the limit as the layer size N tends to infinity. We do not explicitly consider the spectra of the three-or-more particle levels, except to note that generally most of the degeneracy of the unperturbed levels is removed; that which remains is due to the fact that the full and unperturbed matrices have certain symmetries in common.

In Fig. 3 we qualitatively depict the effect of the perturbation $\underline{K}_1(\underline{K}_2 - \underline{I})$ upon the spectrum of $\underline{K}_1$. Note that the two-particle and n-particle levels are

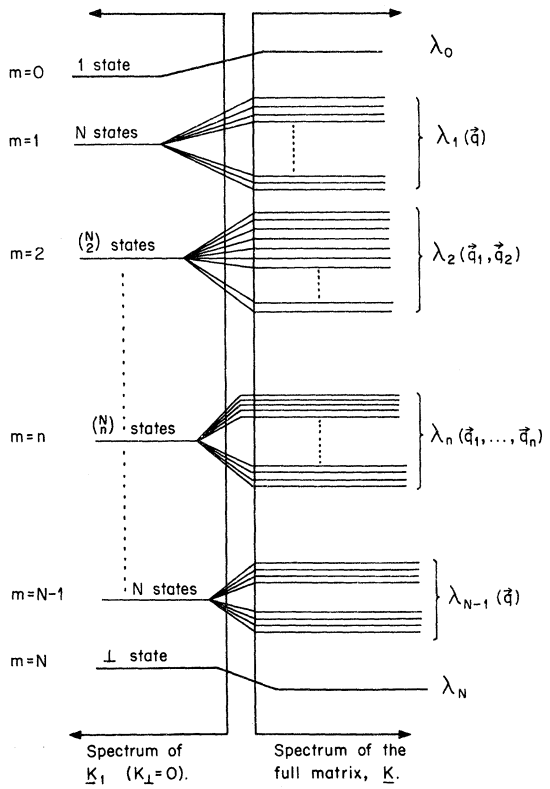

FIG. 3. Spectrum of the transfer matrix $\underline{K}$ at high temperatures. For sufficiently large field h we expect bound states to appear above the bulk of the 2,3,..., n,...-particle bands.

only correctly portrayed for small magnetic fields. For large enough magnetic field, we expect bound states to appear above the continuum bands.

The transfer matrix $\underline{K}$ can easily be expanded in powers of $K_\perp$. Using (2.36) we have

$$\underline{K}=\underline{K}_1+\sum_{n=1}^{\infty}[\underline{K}_1(\underline{K}_2-\underline{I})]_n\,, \tag{3.1}$$

where

$$[\underline{K}_1(\underline{K}_2-\underline{I})]_n=\frac{1}{n!}\,\mu_+^N\exp[-w_{\|}\sum_{\vec{x}}\underline{n}(\vec{x})]\times[\tfrac{1}{2}\sum_{\vec{x},\vec{\delta}}\varphi(\vec{\delta})\underline{\sigma}^z(\vec{x})\underline{\sigma}^z(\vec{x}+\vec{\delta})]^n\,. \tag{3.2}$$

In finding the nth order levels of the single-particle band, we must diagonalize the projection $[\underline{K}_1(\underline{K}_2-\underline{I})]_m$ ($m=1, 2, \ldots, n$), as defined by (3.2), within the single-particle subspace. It would be convenient to know that the same zeroth-order eigenstates diagonalize (3.2) for all n. To show this we make use of the fact that $\{[\underline{K}_1(\underline{K}_2-\underline{I})]_m\}$ are all invariant under the group of translations through the $(d-1)$ primitive lattice vectors of the layer. Thus, any of these operators operating upon a state of definite wave vector $\vec{q}$ ($\vec{q}$ lying upon the lattice reciprocal to the layer lattice) takes it into another state of the same wave vector $\vec{q}$. We say that these operators conserve the layer momentum $\vec{q}$. We can now explicitly show that the same set of states suffices for all n in (3.2). Let $\{|\psi_1(\vec{q})\rangle\}$ be a set of single-particle states of definite $\vec{q}$ such that

$$[\underline{K}_1(\underline{K}_2-\underline{I})]_1\,|\psi_1(\vec{q})\rangle=\Lambda_1(\vec{q})\,|\psi_1(\vec{q})\rangle+|\epsilon(\vec{q})\rangle\,, \tag{3.3}$$

where

$$\langle\psi_1(\vec{q})|\psi_1(\vec{q}\,')\rangle=\delta(\vec{q},\vec{q}\,'),\qquad \langle\psi_1(\vec{q})|\epsilon(\vec{q}\,')\rangle=0\,, \tag{3.4}$$

so that these states diagonalize the projection of $[\underline{K}_1(\underline{K}_2-\underline{I})]_1$ within the single-particle subspace, since by (3.4), $|\epsilon(\vec{q})\rangle$ has no component within the subspace. Now $[\underline{K}_1(\underline{K}_2-\underline{I})]_1|\epsilon(\vec{q})\rangle$, by examination, necessarily has a component in the single-particle subspace. However, since $[\underline{K}_1(\underline{K}_2-\underline{I})]_1$ conserves layer momentum, that component is proportional to $|\psi_1(\vec{q})\rangle$ only. Thus, we have

$$[\underline{K}_1(\underline{K}_2-\underline{I})]_2\,|\psi_1(\vec{q})\rangle=(\mu_+^{1-N}\mu_-^{-1}\{\Lambda_1^2(\vec{q})+\langle\psi_1(\vec{q})|[\underline{K}_1(\underline{K}_2-\underline{I})]_1|\epsilon(\vec{q})\rangle\})\times|\psi_1(\vec{q})\rangle+\mu_+^{1-N}\mu_-^{-1}\Lambda_1(\vec{q})|\epsilon(\vec{q})\rangle\,. \tag{3.5}$$

This is an explicit demonstration that the unitary transformation which diagonalizes $[\underline{K}_1(\underline{K}_2-\underline{I})]_1$ also diagonalizes $[\underline{K}_1(\underline{K}_2-\underline{I})]_2$ within that subspace. By an obvious induction, this may be extended to arbitrary n. A similar proof may be constructed for the m-particle levels.

Since λ_0 is nondegenerate in zeroth order, the calculation of its perturbative corrections is particularly simple and will be presented first. Let

$$\lambda_0=\lambda_0^{(0)}+K_\perp\lambda_0^{(1)}+K_\perp^2\lambda_0^{(2)}+\cdots,\qquad |\lambda_0\rangle=|\lambda_0^{(0)}\rangle+K_\perp|\lambda_0^{(1)}\rangle+\cdots\,; \tag{3.6}$$

then $\lambda_0^{(0)}=\mu_+^N$, and $|\lambda_0^{(0)}\rangle=|\Phi\rangle$, the vacuum state. With the provisions noted in Sec. II, we may take over the formulas of Rayleigh-Schrödinger perturbation theory[20] and apply them to our non-Hermitian operators. If we define $\Upsilon_n^{\pm}$ to be

$$\Upsilon_n^{\pm}=\mu_\pm^n/(\mu_+^n-\mu_-^n)\,, \tag{3.7}$$

then we have

$$K_\perp\lambda_0^{(1)}=\tfrac{1}{2}K_\perp\mu_+^N\sum_{\vec{x},\vec{\delta}}\varphi(\vec{\delta})\langle\Phi|\underline{\sigma}^z(\vec{x})\underline{\sigma}^z(\vec{x}+\vec{\delta})|\Phi\rangle\,, \tag{3.8a}$$

$$K_\perp^2\lambda_0^{(2)}=\tfrac{1}{8}\mu_+^N K_\perp^2\sum_{\vec{x},\vec{\delta}}\sum_{\vec{r},\vec{\gamma}}\varphi(\vec{\delta})\varphi(\vec{\gamma})\times\langle\Phi|\underline{\sigma}^z(\vec{x})\underline{\sigma}^z(\vec{x}+\vec{\delta})\underline{\sigma}^z(\vec{r})\underline{\sigma}^z(\vec{r}+\vec{\gamma})|\Phi\rangle+\tfrac{1}{2}K_\perp^2\mu_+^N\sum_{\vec{x},\vec{\delta}}\varphi(\vec{\delta})\langle\Phi|\underline{\sigma}^z(\vec{x})\underline{\sigma}^z(\vec{x}+\vec{\delta})|\lambda_0^{(1)}\rangle\,, \tag{3.8b}$$

with

$$K_\perp|\lambda_0^{(1)}\rangle=\tfrac{1}{2}K_\perp\sum_{\vec{x},\vec{\delta}}\varphi(\vec{\delta})\sum_{t=1}^{N}\Upsilon_t^-\times\sum_{k=1}^{\binom{N}{t}}|\lambda_{t,k}^{(0)}\rangle\langle\lambda_{t,k}^{(0)}|\underline{\sigma}^z(\vec{x})\underline{\sigma}^z(\vec{x}+\vec{\delta})|\Phi\rangle\,, \tag{3.8c}$$

$$K_\perp\langle\lambda_0^{(1)}|=\tfrac{1}{2}K_\perp\sum_{\vec{x},\vec{\delta}}\varphi(\vec{\delta})\sum_{t=1}^{N}\Upsilon_t^+\times\sum_{k=1}^{\binom{N}{t}}\langle\Phi|\underline{\sigma}^z(\vec{x}+\vec{\delta})\,\underline{\sigma}^z(\vec{x})|\lambda_{t,k}^{(0)}\rangle\langle\lambda_{t,k}^{(0)}|\,, \tag{3.8d}$$

where the states $|\lambda_{t,k}^{(0)}\rangle$ are the $\binom{N}{t}$ states of the degenerate unperturbed level $\lambda_t^{(0)}=\mu_+^{N-t}\mu_-^t$.

The above formulas are easily simplified. Using (2.34) for $\underline{\sigma}^x(\vec{r})$, we see that $\underline{\sigma}^x(\vec{r})\underline{\sigma}^x(\vec{r}+\vec{\delta})$ can lead to transitions which change the particle number by 0, ±1, or ±2 particles. [In zero field, by (2.30), $\underline{\sigma}^x(r)\underline{\sigma}^x(\vec{r}+\vec{\delta})$ can change the particle number only by 0 or ±2 particles.] Thus, in (3.8c) we need only keep the terms with $t=1$ and 2, the other terms being zero by the orthonormality of states with differing particle numbers. For $t=1$, the states $\{|\lambda_1^{(0)}, k\rangle\}$ are the states, labeled $\{|\vec{r}\rangle\}$, of a single particle at layer site $\vec{r}$. Similarly for $t=2$, the states $\{|\lambda_2^{(0)}, k\rangle\}$ are the states called $|\vec{r}_1, \vec{r}_2\rangle$ of two particles at layer sites $\vec{r}_1$ and $\vec{r}_2$. Note that since $(\underline{\psi}^\dagger(\vec{r}))^2$ is zero, there are no states with two particles upon the same layer site.

To simplify our results we introduce the Fourier transform $\hat{\varphi}(\vec{q})$ of the interaction shape function $\varphi(\vec{\delta})$:

$$\hat{\varphi}(\vec{q}) \equiv \sum_{\vec{\delta}} \varphi(\vec{\delta}) e^{i\vec{q}\cdot\vec{\delta}} = \sum_{\vec{\delta}} \varphi(\vec{\delta}) \cos \vec{q}\cdot\vec{\delta} \ , \quad (3.9)$$

where $\vec{q}$ is a reciprocal-lattice vector with $d-1$ components $q_j = 2\pi n_j/N_j$, and n_j runs from 1 to N_j, the number of sites in the jth layer direction. Note that the second equality in (3.9) only holds for layers with a symmetrical lattice structure. If $\varphi(\vec{r})$ equals one for nearest neighbors and zero otherwise, $\hat{\varphi}(\vec{q})$ is referred to as the lattice generating function[5] and $\hat{\varphi}(\vec{0})$ is the layer coordination number—the number of nearest neighbors to a given layer site. The calculation of the matrix elements in (3.8) is straightforwardly performed using the commutation rules (2.25), the expression (2.34) of $\underline{\sigma}^x(\vec{r})$ in terms of the chain creation and annihilation operators, and the single-chain matrix elements given by (2.33). The resulting formulas for the largest level (assuming periodic boundary conditions within the layer) are

$$\lambda_0 = \mu_+^N \{1 + \tfrac{1}{2}K_\perp N\hat{\varphi}(\vec{0}) S_{++}^2 + \tfrac{1}{8}K_\perp^2 \{ S_{++}^4 [N^2\hat{\varphi}(\vec{0})^2 - 4N\hat{\varphi}(\vec{0})^2 + 2N\hat{\varphi}(\vec{0})]$$
$$+ S_{++}^2 [4N\hat{\varphi}(\vec{0})^2] + 2N\hat{\varphi}(\vec{0})\} + K_\perp^2 \{ \Upsilon_1^- N\hat{\varphi}(\vec{0})^2 S_{-+}^2 S_{++}^2 + \tfrac{1}{2} N\hat{\varphi}(\vec{0}) \Upsilon_2^- |S_{+-}|^4\} + O(K_\perp^3)) \ , \quad (3.10a)$$

$$|\lambda_0\rangle = |\Phi\rangle + K_\perp \hat{\varphi}(\vec{0}) S_{-+} S_{++} \Upsilon_1^- \sum_{\vec{r}} |\vec{r}\rangle + \tfrac{1}{2} K_\perp S_{-+}^2 \Upsilon_2^- \sum_{\vec{r},\vec{\delta}} \varphi(\vec{\delta}) |\vec{r}, \ \vec{r}+\vec{\delta}\rangle + O(K_\perp^2) \ , \quad (3.10b)$$

$$\langle\lambda_0| = \langle\Phi| + K_\perp \hat{\varphi}(\vec{0}) S_{+-} S_{++} \Upsilon_1^+ \sum_{\vec{r}} \langle\vec{r}| + \tfrac{1}{2} K_\perp S_{+-}^2 \Upsilon_2^+ \sum_{\vec{r},\vec{\delta}} \hat{\varphi}(\vec{\delta}) \langle \vec{r}, \ \vec{r}+\vec{\delta}| \ , \quad (3.10c)$$

where the effect of non-Hermiticity of $\underline{K}$ is seen in the replacement of Υ_n^- in (3.10b) by $\overline{\Upsilon_n^+}$ in (3.10c). In zero field we have $S_{++} = S_{--} = 0$ and $S_{+-} = S_{-+} = 1$; furthermore, $\Upsilon_2^+ = \cosh^2 K_\parallel$ and $\Upsilon_2^- = \sinh^2 K_\parallel$. The free energy per site $-\beta f_c$ was shown in I to be $N^{-1} \ln \lambda_0$.[1] Thus, to second order in $K_\perp$, we have

$$-\beta f_c = \ln 2 + \ln \cosh K_\parallel + \tfrac{1}{4} K_\perp^2 \hat{\varphi}(\vec{0}) \{1 + 2\sinh^2 K_\parallel\} + O(K_\perp^3) \ . \quad (3.11)$$

This result agrees with that obtained from exact series expansions, as presented by Fisher.[21]

For the single-particle band, we shall find that $[\underline{K}_1(\underline{K}_2 - \underline{I})]_1$ breaks the N-fold degeneracy of the states of given wave vector $\vec{q}$ with components, as given above, $q_i = 2\pi n_i/N_i$, $i = 1, 2, \ldots, d-1$. (Recall that $N = N_1 N_2 \cdots N_{d-1}$, where N_p is the number of sites in the pth layer direction.) As above, we assume cyclic boundary conditions within the layers.

From degenerate perturbation theory[20] we know that the first-order single-particle eigenvalues are obtained by diagonalizing the matrix $M_1(\vec{r}, \vec{r}')$ defined by

$$M_1(\vec{r}, \vec{r}') \equiv \langle \vec{r}\,| [\underline{K}_1(\underline{K}_2 - \underline{I})]_1 |\vec{r}\,'\rangle = \tfrac{1}{2} K_\perp \mu_+^{N-1} \mu_- \sum_{\vec{\delta}} \varphi(\vec{\delta}) \langle \vec{r}\,| \underline{\sigma}^x(\vec{x}) \underline{\sigma}^x(\vec{x}+\vec{\delta}) |\vec{r}\,'\rangle \ . \quad (3.12)$$

A word about boundary conditions is appropriate. With free-edge boundary conditions, every layer vector $\vec{x}$ is written $\vec{x} = (x_1, x_2, \ldots, x_{d-1})$ and verifies

$$1 \le x_m \le N_m \quad (m = 1, 2, \ldots, d-1) \ , \quad (3.13)$$

for every function of the layer vector $\vec{x}$. Whereas periodic boundary conditions lead to running-wave single-particle states, we shall find in Paper IV that free-edge boundary conditions lead to standing waves.

The N states $\{|\vec{r}\rangle\}$ form an orthonormal basis for the single-particle subspace, so we may use the completeness relation

$$\underline{I}_1 = \sum_{\vec{r}} |\vec{r}\rangle\langle\vec{r}| \ , \quad (3.14)$$

where $\underline{I}_1$ is the projection of the identity onto the single-particle subspace. Let the (undetermined) linear combination of single-particle states which diagonalizes $[\underline{K}_1(\underline{K}_2 - \underline{I})]_1$ be labeled $|\vec{q}\rangle$; then using (3.14) we may write

$$\langle\vec{q}\,| [\underline{K}_1(\underline{K}_2 - \underline{I})]_1 |\vec{q}\,'\rangle = \sum_{\vec{r},\vec{r}'} \langle\vec{q}\,|\vec{r}\rangle M_1(\vec{r}, \vec{r}\,') \langle \vec{r}\,'|\vec{q}\,'\rangle \ . \quad (3.15)$$

Thus, we need to find the unitary matrix $\langle\vec{r}\,|\vec{q}\rangle \equiv \phi_{\vec{q}}(\vec{r})$ which diagonalizes $M_1(\vec{r}, \vec{r}\,')$. The elements $\{\phi_{\vec{q}}(\vec{r})\}$ are clearly the wave functions of $|\vec{q}\rangle$ in the $\vec{r}$ representation.

As mentioned above, we assume that $\{\phi_{\vec{q}}(\vec{r})\}$ are running waves within the layer,

$$\phi_{\vec{q}}(\vec{r}) = N^{-1/2} e^{i\vec{q}\cdot\vec{r}} = N^{-1/2} \exp\left(2\pi i \sum_{j=1}^{d-1} n_j r_j/N_j\right) \ , \quad (3.16)$$

where n_j runs from 1 to N_j. The following fundamental equation is easily proven and very useful:

$$\sum_{x=1}^{N} e^{2\pi i k x/N} = N\delta(k, 0) = N\delta(k, N) \ , \quad (3.17)$$

where k is restricted to $1, 2, \ldots, N$.

Using (3.17), orthonormality of $\{|\vec{q}\rangle\}$ is easily proven. Consider $\langle\vec{q}\,|\vec{q}\,'\rangle$:

$$\langle \vec{q}|\vec{q}'\rangle = \sum_{\vec{r}} \phi^*_{\vec{q}}(\vec{r})\,\phi_{\vec{q}'}(\vec{r}) = (N_1\cdots N_{d-1})^{-1} \sum_{r_1=1}^{N_1}\cdots\sum_{r_{d-1}=1}^{N_{d-1}} \exp\left(2\pi i \sum_{j=1}^{d-1}\frac{(n_j'-n_j)r_j}{N_j}\right) . \tag{3.18}$$

We may apply (3.17) to each component of (3.18), so that

$$\langle \vec{q}|\vec{q}'\rangle = \delta(n_1,n_1')\cdots\delta(n_{d-1},n_{d-1}') \equiv \delta(\vec{q},\vec{q}') . \tag{3.19}$$

This proves orthonormality. To prove completeness, we need only show that $\langle \vec{r}|\vec{r}'\rangle = \delta(\vec{r},\vec{r}')$ is preserved in the $\{|\vec{q}\rangle\}$ representation, the set $\{|\vec{r}\rangle\}$ being itself complete. Thus, we examine

$$\sum_{\vec{q}}\langle \vec{r}|\vec{q}\rangle\langle\vec{q}|\vec{r}'\rangle = \sum_{\vec{q}}\phi^*_{\vec{q}}(\vec{r})\,\phi_{\vec{q}}(\vec{r}')$$

$$= (N_1\cdots N_{d-1})^{-1}\sum_{n_1=1}^{N_1}\cdots\sum_{n_{d-1}=1}^{N_{d-1}} \times\exp\left(2\pi i\sum_{j=1}^{d-1}\frac{n_j(r_j'-r_j)}{N_j}\right). \tag{3.20}$$

From (3.17) we again see that

$$\sum_{\vec{q}}\langle\vec{r}|\vec{q}\rangle\langle\vec{q}|\vec{r}'\rangle = \delta(r_1,r_1')\cdots\delta(r_{d-1},r_{d-1}') \equiv \delta(\vec{r},\vec{r}') , \tag{3.21}$$

so that $\{|\vec{q}\rangle\}$ forms a complete orthonormal basis for the single-particle subspace.

Application of this running-wave transformation to $M_1(\vec{r},\vec{r}')$ yields the diagonal form

$$\langle\vec{q}|[\underline{K}_1(\underline{K}_2-\underline{I})]_1|\vec{q}'\rangle = \delta(\vec{q},\vec{q}')\tfrac{1}{2}K_\perp\mu_+^{N-1}\mu_- \times\{[(N-2)\hat{\varphi}(\vec{0})S_{++}^2 + 2S_{++}S_{--}] + 2|S_{+-}|^2\hat{\varphi}(\vec{q})\} , \tag{3.22}$$

where $\hat{\varphi}(\vec{q})$ is given by (3.9). This shows $\{|\vec{q}\rangle\}$ to be the N zeroth-order single-particle eigenstates of $\underline{K}$. Notice that not all the degeneracy has been broken, in particular, the replacement of any component q_j of $\vec{q}$ by $2\pi - q_j$ leaves $\lambda_1(\vec{q})$ unchanged. This corresponds to the natural degeneracy of running waves traveling to the left or the right in a given direction. Since the degeneracy arises because of a common symmetry of $\underline{K}_1$ and $[\underline{K}_1(\underline{K}_2-\underline{I})]_n$ for all n, higher-order terms will also fail to mix these states, and we may ignore this degeneracy in obtaining higher-order corrections to $\lambda_1(\vec{q})$ and $|\lambda_1(\vec{q})\rangle$.

The calculation of $\lambda_1(\vec{q})$ to second order in $K_\perp$ and of $|\lambda_1(\vec{q})\rangle$ to first order in $K_\perp$ is straightforward but tedious. Thus, we only state the results here:

$$|\lambda_1(\vec{q})\rangle = N^{-1/2}\sum_{\vec{r}} e^{i\vec{q}\cdot\vec{r}}\Big(|\vec{r}\rangle + K_\perp\{-\hat{\varphi}(\vec{0})\Upsilon_1^+ S_{++}S_{+-}|\Phi\rangle + \Upsilon_1^-[S_{-+}(S_{--}-S_{++})\sum_{\vec{\delta}}\varphi(\vec{\delta})|\vec{r},\vec{r}+\vec{\delta}\rangle + \hat{\varphi}(\vec{0})S_{-+}S_{+-}\sum_{\vec{r}_1}|\vec{r},\vec{r}_1\rangle] + \tfrac{1}{2}\Upsilon_2^- S_{-+}^2\sum_{\vec{r}_1}\sum_{\vec{\delta}}\varphi(\vec{\delta})|\vec{r},\vec{r}_1,\vec{r}_1+\vec{\delta}\rangle\}\Big) + O(K_1^2) , \tag{3.23a}$$

$$\lambda_1(\vec{q}) = \mu_+^{N-1}\mu_-\Big[1+\tfrac{1}{2}K_\perp\{[(N-2)S_{++}^2\hat{\varphi}(\vec{0}) + 2S_{--}S_{++}] + 2|S_{+-}|^2\hat{\varphi}(\vec{q})\} + K_\perp^2\Big(\Upsilon_1^-\{(N-2)\hat{\varphi}(\vec{0})S_{++}^2|S_{+-}|^2 + [1+\hat{\varphi}(\vec{q})][|S_{+-}|^2(S_{--}^2-S_{++}^2) + 2\hat{\varphi}(\vec{0})|S_{+-}|^2 S_{++}(S_{--}-S_{++})]\} + \tfrac{1}{2}\Upsilon_2^-|S_{-+}|^4[(N-4)\hat{\varphi}(\vec{0}) + 2\hat{\varphi}^2(\vec{q})]\Big) + \tfrac{1}{8}K_\perp^2\Big(2N\hat{\varphi}(\vec{0}) + 8S_{--}S_{++}\hat{\varphi}(\vec{0})[\hat{\varphi}(\vec{0})-1] + 4(N-2)S_{++}^2\hat{\varphi}(\vec{0})[\hat{\varphi}(\vec{0})-1] + 8|S_{+-}|^2[\hat{\varphi}(\vec{q})^2 - \hat{\varphi}(\vec{0})] + S_{++}^3(S_{--}-S_{++})[4N\hat{\varphi}(\vec{0})^2 + 8\hat{\varphi}(\vec{0}) - 16\hat{\varphi}(\vec{0})^2] + S_{++}^4[N^2\hat{\varphi}(\vec{0})^2 - 4N\hat{\varphi}(\vec{0})^2 + 2N\hat{\varphi}(\vec{0})] + 4S_{++}^2|S_{+-}|^2\{-2\hat{\varphi}(\vec{0})^2 + [(N-8)\hat{\varphi}(\vec{0}) + 4]\hat{\varphi}(\vec{q}) - 2[\hat{\varphi}(\vec{q})^2 - \hat{\varphi}(\vec{0})]\}\Big) + O(K_\perp^3)\Big]. \tag{3.23b}$$

Again these results are very much simplified in the zero-field limit. We remark that $\langle\lambda_1(\vec{q})|$ is obtained from (3.23a) by changing all ket vectors to bra vectors, interchanging S_{+-} and S_{-+} and interchanging Υ_n^- and Υ_n^+.

In our consideration of the two-particle band, we shall find that only in two dimensions are we able to obtain the zeroth-order eigenstates for arbitrary layer size N. In three or more dimensions we are able to obtain the states in the limit as N tends to infinity.

Our unperturbed states are $|\vec{r}_1,\vec{r}_2\rangle = \underline{\psi}^\dagger(\vec{r}_1)\times\underline{\psi}^\dagger(\vec{r}_2)|\Phi\rangle$. These states have the properties that only a single particle may occupy a given site and that the states are even under interchange of particle coordinates. Thus, for the $N(N-1)$ combinations of $\vec{r}_1$ and $\vec{r}_2$ with $\vec{r}_1\neq\vec{r}_2$, there are only $\frac{1}{2}N(N-1)$ distinct states because such an enumer-

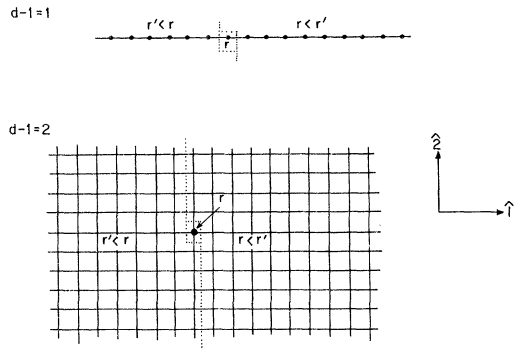

FIG. 4. "Dictionary ordering" for the two-particle states.

ation counts each state twice.

It will be useful for our work below if we introduce a labeling convention for the lattice sites of a layer. We say that $\vec{r}_1 < \vec{r}_2$, if

(i) $r_{1,1} < r_{2,1}$; or
(ii) $r_{1,1} = r_{2,1}$ and $r_{1,2} < r_{2,2}$; or
(iii) $r_{1,1} = r_{2,1}, r_{1,2} = r_{2,2}$, and $r_{1,3} < r_{2,3}$; or...
$(d-1)$ $r_{1,1} = r_{2,1}, r_{1,2} = r_{2,2}, \cdots, r_{1,d-2} = r_{2,d-2}$, and

$$r_{1,d-1} < r_{2,d-1} , \quad (3.24)$$

where $r_{1,j}$ and $r_{2,j}$ are the components of $\vec{r}_1$ and $\vec{r}_2$, respectively, in the jth lattice direction. In Fig. 4, we illustrate this convention for two- and three-dimensional systems (one- and two-dimensional layers). Note that this labeling convention generates all the distinct states of two particles on the lattice. That is, we have

$$\underline{I}_2 = \sum_{\vec{r}_1 < \vec{r}_2} |\vec{r}_1, \vec{r}_2\rangle\langle\vec{r}_1, \vec{r}_2| , \quad (3.25)$$

where $\underline{I}_2$ is the projection of the identity onto the two-particle subspace.

The determination of the two-particle spectrum to first order in $K_\perp$ involves only the breaking of the degeneracy of the $\frac{1}{2}N(N-1)$ states $\{|\vec{r}_1, \vec{r}_2\rangle\}$ via the diagonalization of the perturbation operator $[\underline{K}_1(\underline{K}_2 - \underline{I})]_1$ within the two-particle subspace. We do so by searching for a set of two-particle states $\{|\Psi(\vec{q}_1, \vec{q}_2)\rangle\}$ which are those linear combinations of $\{|\vec{r}_1, \vec{r}_2\rangle\}$ that are eigenstates of the particle-number conserving terms in $[\underline{K}_1(\underline{K}_2 - \underline{I})]_1$. As noted above, this problem turns out to be isomorphic to that of finding the two-spin deviation states for the X-Y model.[23]

We may write the particle-number conserving part of $[\underline{K}_1(\underline{K}_2 - \underline{I})]_1$ in zero field as

$$\mathcal{H}_c = \mu_+^N \exp[-w_\parallel \sum_{\vec{x}} \underline{n}(\vec{x})] \tfrac{1}{2} K_\perp \sum_{\vec{x},\vec{\delta}} [\underline{\psi}^\dagger(\vec{x})\underline{\psi}(\vec{x}+\vec{\delta}) + \underline{\psi}(\vec{x})\underline{\psi}^\dagger(\vec{x}+\vec{\delta})] . \quad (3.26)$$

We now construct a complete orthonormal set of states which are the exact eigenstates of $\mathcal{H}_c$ for arbitrary N in two dimensions and which, in three or more dimensions, are asymptotically the exact eigenstates as N tends to infinity.

Consider the following set of states $\{|\Psi(\vec{q}_1, \vec{q}_2)\rangle\}$:

$$|\Psi(\vec{q}_1, \vec{q}_2)\rangle = \sum_{\vec{r}_1} \sum_{\vec{r}_2} \Psi_{\vec{q}_1\vec{q}_2}(\vec{r}_1, \vec{r}_2) |\vec{r}_1, \vec{r}_2\rangle , \quad (3.27)$$

where $\vec{q}_1$ and $\vec{q}_2$ are wave vectors defined below and $\Psi_{\vec{q}_1\vec{q}_2}(\vec{r}_1, \vec{r}_2)$ is defined as follows. Let $\mathrm{sgn}(\vec{x}, \vec{y})$ be defined as

$$\mathrm{sgn}(\vec{x}, \vec{y}) = \begin{cases} +1, & \vec{x} < \vec{y} \\ -1, & \vec{x} > \vec{y} \end{cases} \quad (3.28)$$

where by $\overset{<}{>}$ we mean our "dictionary ordering" introduced in (3.24). Then $\Psi_{\vec{q}_1\vec{q}_2}(\vec{r}_1, \vec{r}_2)$ is given by

$$\Psi_{\vec{q}_1\vec{q}_2}(\vec{r}_1, \vec{r}_2) = \mathrm{sgn}(\vec{q}_1, \vec{q}_2)\ \mathrm{sgn}(\vec{r}_1, \vec{r}_2) \times \tfrac{1}{2}[\exp(i\vec{q}_1\cdot\vec{r}_1 + i\vec{q}_2\cdot\vec{r}_2) - \exp(i\vec{q}_1\cdot\vec{r}_2 + i\vec{q}_2\cdot\vec{r}_1)] . \quad (3.29)$$

With this definition, the wave function $\Psi_{\vec{q}_1\vec{q}_2}(\vec{r}_1, \vec{r}_2)$ is symmetrical under exchange of both $\vec{r}_1$ and $\vec{r}_2$, and $\vec{q}_1$ and $\vec{q}_2$. In addition, we have $\Psi_{\vec{q}_1\vec{q}_2}(\vec{r}_1, \vec{r}_1) = \Psi_{\vec{q}_1\vec{q}_1}(\vec{r}_1, \vec{r}_2) = 0$. Orthonormality is easily proven. Indeed, we have

$$\langle\Psi(\vec{q}_1, \vec{q}_2)|\Psi(\vec{q}_1', \vec{q}_2')\rangle = \begin{cases} \delta(\vec{q}_1, \vec{q}_1')\,\delta(\vec{q}_2, \vec{q}_2'), & \vec{q}_1 \lesseqgtr \vec{q}_2,\ \vec{q}_1' \lesseqgtr \vec{q}_2' \\ \delta(\vec{q}_1, \vec{q}_2')\,\delta(\vec{q}_2, \vec{q}_1'), & \vec{q}_1 \lesseqgtr \vec{q}_2,\ \vec{q}_1' \gtreqless \vec{q}_2' \end{cases} . \quad (3.30)$$

Now (3.30) is valid for both cyclic and anticyclic boundary conditions, that is, if the components of $\vec{q}$ are q_j, then (3.30) holds for both $q_j = 2\pi n_j/N_j$ and $q_j = (2n_j+1)\pi/N_j$, with n_j an integer $1, 2, \ldots, N_j$. It is easily seen that the requirement that $|\Psi(\vec{q}_1, \vec{q}_2)\rangle$ be continuous across a zone boundary means that we need choose the anticyclic boundary conditions.[23] Of course, the choice of boundary conditions becomes irrelevant in the limit as $N_1, N_2, \ldots, N_{d-1}$ tend to infinity.

We now consider the effect of $\mathcal{H}_c$ upon $|\Psi(\vec{q}_1, \vec{q}_2)\rangle$:

$$\mathcal{H}_c|\Psi(\vec{q}_1, \vec{q}_2)\rangle = K_\perp \mu_+^{N-2} \mu_-^2 \sum_{\vec{\delta}} \varphi(\vec{\delta})[\cos(\vec{q}_1\cdot\vec{\delta}) + \cos(\vec{q}_2\cdot\vec{\delta})] \times \sum_{\vec{r}_2+\vec{\delta} < \vec{r}_1 < \vec{r}_2-\vec{\delta}} \Psi_{\vec{q}_1\vec{q}_2}(\vec{r}_1, \vec{r}_2)|\vec{r}_1, \vec{r}_2\rangle . \quad (3.31)$$

Upon rearrangement of terms we find that

$$[\mu_+^{N-2}\mu_-^2]^{-1}\{\mathcal{H}_c - K_\perp \mu_+^{N-2}\mu_-^2[\hat{\varphi}(\vec{q}_1) + \hat{\varphi}(\vec{q}_2)]\}|\Psi(\vec{q}_1, \vec{q}_2)\rangle = |\zeta(\vec{q}_1, \vec{q}_2)\rangle , \quad (3.32)$$

with

$$|\zeta(q_1, q_2)\rangle = -K_\perp \sum_{\vec{\delta}} \varphi(\vec{\delta})[\cos\vec{q}_1\cdot\vec{\delta} + \cos\vec{q}_2\cdot\vec{\delta}] \sum_{\vec{r}_2-\vec{\delta}<\vec{r}_1<\vec{r}_2+\vec{\delta}} \Psi_{\vec{q}_1\vec{q}_2}(\vec{r}_1, \vec{r}_2)|\vec{r}_1, \vec{r}_2\rangle \ . \tag{3.33}$$

In two dimensions the layers are one dimensional. From Fig. 4 we see that in this case the inequalities $r_1 < r_2 \pm 1$ and $r_1 > r_2 \mp 1$ can never be satisfied simultaneously. Therefore, with $d = 2$ and nearest-neighbor forces, $|\zeta(\vec{q}_1, \vec{q}_2)\rangle$ is identically zero; and by (3.31) $\{|\Psi(\vec{q}_1, \vec{q}_2)\rangle\}$ are seen to be the zeroth-order eigenstates of $\underline{K}$ for arbitrary N. However, by examination of Fig. 4, we see that in three or more dimensions there are, given $\vec{r}_2$, $O(N^{(d-2)/(d-1)})$ sites $\vec{r}_1$ which simultaneously satisfy $\vec{r}_2 - \vec{\delta} < \vec{r}_1 < \vec{r}_2 + \vec{\delta}$. Therefore, in these cases, $|\Psi(\vec{q}_1, \vec{q}_2)\rangle$ are not the zeroth-order eigenstates for finite N.

The norm $\|\zeta(\vec{q}_1, \vec{q}_2)\|$ of $|\zeta(\vec{q}_1, \vec{q}_2)\rangle$ is defined by

$$\|\zeta(\vec{q}_1, \vec{q}_2)\| = [\langle\zeta(\vec{q}_1, \vec{q}_2)|\zeta(\vec{q}_1, \vec{q}_2)\rangle]^{1/2} \ . \tag{3.34}$$

Using (3.33) and the orthonormality of $\{|\vec{r}_1, \vec{r}_2\rangle\}$, we have

$$\|\zeta(\vec{q}_1, \vec{q}_2)\|^2 = K_\perp^2 \sum_{\vec{\delta}} [\hat{\varphi}(\vec{q}_1) + \hat{\varphi}(\vec{q}_2)]\varphi(\vec{\delta}) \times \sum_{\vec{r}_2-\vec{\delta}<\vec{r}_1<\vec{r}_2+\vec{\delta}} 2(\cos\vec{q}_1\cdot\vec{\delta} + \cos\vec{q}_2\cdot\vec{\delta})|\Psi_{\vec{q}_1\vec{q}_2}(\vec{r}_1, \vec{r}_2)|^2 \ . \tag{3.35}$$

This equation may be further reduced; however, there is no need to do so. For, noting that $|\Psi_{\vec{q}_1\vec{q}_2}(\vec{r}_1, \vec{r}_2)|^2 = O(N^{-2})$ and that there are $O(N^{(2d-3)/(d-1)})$ terms in the summation in (3.35), we have found that

$$\|\zeta(\vec{q}_1, \vec{q}_2)\|^2 = O(N^{-1/(d-1)}), \quad N \to \infty \ . \tag{3.36}$$

Thus, in the limit as N tends to infinity, $\|\zeta(\vec{q}_1, \vec{q}_2)\|$ tends to zero. But, we know that the norm of a vector is zero, if and only if the vector is itself null.[24] Thus, as N tends to infinity, the right-hand side of (3.32) tends to zero. So in this limit we have

$$|\lambda_2(\vec{q}_1, \vec{q}_2)\rangle = |\Psi(\vec{q}_1, \vec{q}_2)\rangle + O(K_\perp) \ , \tag{3.37a}$$

$$\lambda_2(\vec{q}_1, \vec{q}_2) = \mu_+^{N-2}\mu_-^2\{1 + K_\perp[\hat{\varphi}(\vec{q}_1) + \hat{\varphi}(\vec{q}_2)] + O(K_\perp^2)\} \ , \tag{3.37b}$$

where $\{|\lambda_2(\vec{q}_1, \vec{q}_2)\rangle\}$ and $\{\lambda_2(\vec{q}_1, \vec{q}_2)\}$ are the two-particle eigenvectors and eigenvalues of $\underline{K}$.

Thus, we have obtained the low-order spectrum of the two-particle level in zero field as N tends to infinity. By an exactly analogous procedure we can calculate the low-order eigenvalues and eigenvectors of the n-particle level for any finite n in the same limit. The zeroth-order states are symmetrized Slater determinants of running waves and the eigenvalues are found to be

$$\lambda_n(\vec{q}_1, \ldots, \vec{q}_n) = \mu_+^{N-n}\mu_-^n[1 + K_\perp \sum_{j=1}^{n} \hat{\varphi}(\vec{q}_j) + O(K_\perp^2)] \ . \tag{3.38}$$

It is straightforward to consider the analogous problem in a finite field. However, in that case, we are confronted with quartic interactions as found in the Heisenberg model. One then expects the appearance of two-particle bound states which may have eigenvalues above the remainder of the band. This point has been fully discussed for the Heisenberg model by Wortis.[23] (However, treating these field-dependent terms as a perturbation on the $N = \infty$, zero-field levels, no evidence of anomalous shifts indicative of bound states appears in leading order.) In any case, as noted above, in a finite field the two-particle levels are of limited importance—entering neither the thermodynamics nor the leading term in the asymptotic decay of correlations.

Summary of II and III

Sections II and III have been largely computational in character. In obtaining the largest eigenvalues of the transfer matrix spectrum at high temperatures, we have garnered the tools necessary to an analysis of the decay of correlation functions at high temperatures.

The qualitative aspects of the spectrum are depicted in Fig. 3. The basis for our calculations is (2.14), which gives the transfer matrix in a form suitable for development in either a high-temperature (small $K_\perp$) series or a low-temperature (small $u_\parallel$) series. The low-temperature variable $u_\parallel$ has completely disappeared from our formulas (2.31) and (2.36)—the suitable high-temperature expressions for $\underline{K}$.

The cyclic spectrum is examined in Sec. III. The important results are (3.10a)–(3.10c) for the largest (and most important) level, (3.23a) and (3.23b) for the single-particle levels, and (3.27), (3.29), (3.37a), and (3.37b) for the zero-field two-particle levels.

IV. DECAY OF SPIN CORRELATION FUNCTIONS

From Paper I, we recall that the asymptotic decay of correlation functions is determined by the largest level and the first band below it (the single-particle band), if the appropriate matrix elements are nonzero. Consider the correlation between spins at sites $\vec{R}_0$ and $\vec{R}_0 + \vec{R}$, where $\vec{R} = \vec{r}_\perp + \hat{z}r_\parallel$ and both $\vec{R}_0$ and $\vec{R}_0 + \vec{R}$ are far from any surfaces:

$$G_s(\vec{R}) \equiv \langle \delta S^z(\vec{R}_0)\,\delta S^z(\vec{R}_0 + \vec{R})\rangle. \tag{4.1}$$

Then according to (3.46) and (3.48) we have

$$G_s(\vec{R}) \approx \sum_{\vec{q}} \left(\frac{\lambda_1(\vec{q})}{\lambda_0}\right)^{|r_\parallel|} \langle\lambda_0|\sigma^z(\vec{0})|\lambda_1(\vec{q})\rangle\langle\lambda_1(\vec{q})|\sigma^z(\vec{r}_\perp)|\lambda_0\rangle$$

$$\text{as } |r_{\parallel}| \to \infty. \qquad (4.2)$$

We define the wave-vector dependent inverse length $\hat{\kappa}(\vec{q})$ as

$$\hat{\kappa}(\vec{q}) \equiv \ln\lambda_0 - \ln\lambda_1(\vec{q}) \,. \qquad (4.3)$$

Then the inverse range of correlation κ defined by (3.47) and (3.49) of Paper I is found to be $\hat{\kappa}(\vec{q}=0)$. To first order in $K_\perp$, $\hat{\kappa}(\vec{q})$ may be written, using (3.10a) and (3.23b),

$$\hat{\kappa}(\vec{q}) = \ln(\mu_+/\mu_-) - K_\perp[\hat{\varphi}(\vec{0})S_{++}(S_{--} - S_{++}) + |S_{+-}|^2\,\hat{\varphi}(\vec{q})] + O(K_\perp^2), \qquad (4.4)$$

which becomes, in zero field,

$$\hat{\kappa}(\vec{q}) = \ln(\coth K_{\parallel}) - K_\perp\hat{\varphi}(\vec{q}) + O(K_\perp^2). \qquad (4.5)$$

Our calculations of λ_0 and $\lambda_1(\vec{q})$ actually enable us to write $\hat{\kappa}(\vec{q})$ to second order in $K_\perp$. However, for finite wave vector $\vec{q}$ and/or magnetic field h, the expression is cumbersome. Thus, we present only $\kappa = \hat{\kappa}(\vec{q}=0)$ for $h=0$ to second order in $K_\perp$:

$$\kappa = \ln(\coth K_{\parallel}) - \hat{\varphi}(\vec{0})K_\perp - \tfrac{1}{2}K_\perp^2\{[\hat{\varphi}^2(\vec{0}) - 2\,\hat{\varphi}(\vec{0})](2\cosh^2 K_{\parallel} - 1)\} + O(K_\perp^3). \qquad (4.6)$$

For $d=2$ and nearest-neighbor forces $\hat{\varphi}(\vec{0}) = 2$, κ reduces to

$$\kappa = \ln[\coth(K_{\parallel})] - 2K_\perp + O(K_\perp^3) \quad (d=2,\ h=0), \qquad (4.7)$$

in agreement with Onsager's exact result.[14] For the zero-field simple cubic nearest-neighbor model we have $\hat{\varphi}(\vec{0}) = 4$; and we find

$$\kappa = \ln[\coth(K_{\parallel})] - 4K_\perp^2 + O(K^3), \qquad (4.8)$$

in agreement with the high-temperature series expansion of Fisher and Burford.[5] For finite fields, κ has never previously been calculated, so we have no check for our finite-field results.

There exists a problem with our calculation of $\hat{\kappa}(\vec{q})$, namely, we have not shown that $\hat{\kappa}(\vec{q})$ tends to a finite limit as N tends to infinity. In the formulas for κ and $\hat{\kappa}(\vec{q})$ given above, the N dependences of $\lambda_0(N)$ and $\lambda_1(\vec{q}, N)$ have exactly canceled. The eigenvalues λ_0 and $\lambda_1(\vec{q})$ are like reduced partition functions, and we expect that they may be written as N tends to infinity as $\exp\{-N\beta f\}$ and $\exp\{-[N\beta f + F_1(\vec{q})]\}$, respectively, where f is the free-energy density and $F_1(\vec{q})$ is N dependent. In order that $\hat{\kappa}(\vec{q})$ be finite, $F_1(\vec{q})$ must tend to a constant (or zero, as at a critical point) as N tends to infinity. Although we have not made any attempt to prove that this in fact occurs, experience with such many-body expansions and the exact two-dimensional results leave us no doubt that our expansion for $\hat{\kappa}(\vec{q})$ has a finite radius of convergence in the $K_\perp$ plane in the limit as N tends to infinity.[25]

Given as expression for $\hat{\kappa}(\vec{q})$, the calculation of $G_s(\vec{R})$ rests upon the matrix elements

$$M(\vec{q}, \vec{r}_\perp) = \langle\lambda_1(\vec{q})\,|\,\underline{\sigma}^z(\vec{r}_\perp)\,|\,\lambda_0\rangle\,, \qquad \tilde{M}(\vec{q}, \vec{r}_\perp) = \langle\lambda_0\,|\,\underline{\sigma}^z(\vec{r}_\perp)\,|\,\lambda_1(\vec{q})\rangle\,. \qquad (4.9)$$

From (2.34), (3.10b), (3.10c), and (3.23a) we obtain

$$M(\vec{q}, \vec{r}_\perp) = N^{-1/2}e^{-i\vec{q}\cdot\vec{r}_\perp}[S_{-+} + K_\perp\,[\Upsilon_1^- S_{-+}S_{++}S_{--}\,\hat{\varphi}(0) + S_{++}^2 S_{+-}\Upsilon_2^-\hat{\varphi}(\vec{q})] + O(K_\perp^2)], \qquad (4.10)$$

from which we obtain $\tilde{M}(\vec{q}, \vec{r}_\perp)$ by complex configuration and replacement of Υ_n^- by Υ_n^+. With (4.10) we re-express $G_s(\vec{R})$ as

$$G_s(\vec{R}) \approx N^{-1}\sum_{\vec{q}}\exp[-\hat{\kappa}(\vec{q})\,|r_{\parallel}| - i\vec{q}\cdot\vec{r}_\perp]\,|S_{+-}|^2\{1 + K_\perp[\hat{\varphi}(\vec{0})S_{++}S_{--}(\Upsilon_1^+ + \Upsilon_1^-) + |S_{+-}|^2(\Upsilon_2^+ + \Upsilon_2^-)\,\hat{\varphi}(\vec{q})] + O(K_\perp^2)\} \quad \text{as } |r_{\parallel}| \to \infty. \qquad (4.11)$$

Recall that $\vec{q}$ is given by

$$(2\pi n_1/N_1,\ 2\pi n_2/N_2,\ 2\pi n_3/N_3, \cdots, 2\pi n_{d-1}/N_{d-1}),$$

where n_j ranges from 1 to N_j for $j = 1, 2, \ldots, d-1$; and also that $N = N_1N_2\cdots N_{d-1}$, so that as N_j tends to infinity, q_j tends to a continuous variable with range $(0, 2\pi)$. The sum over $\vec{q}$ may be written

$$\frac{1}{N}\sum_{\vec{q}} h(\vec{q}) = \frac{1}{N_1}\sum_{n_1=1}^{N_1}\cdots\frac{1}{N_{d-1}}\sum_{N_{d-1}=1}^{N_{d-1}} h\left(\frac{2\pi n_1}{N_1}, \frac{2\pi n_2}{N_2}, \ldots, \frac{2\pi n_{d-1}}{N_{d-1}}\right)\,. \qquad (4.12)$$

So, as N tends to infinity, the sum (4.12) defines a Riemann integral over a $(d-1)$-dimensional hypercubical domain of volume 1. That is,

$$\lim_{N_1\to\infty}\cdots\lim_{N_{d-1}\to\infty}\frac{1}{N}\sum_{\vec{q}} h(\vec{q})$$

$$= \int_0^{2\pi} \frac{dq_1}{2\pi} \cdots \int_0^{2\pi} \frac{dq_{d-1}}{2\pi} h(q_1, \ldots q_{d-1}), \quad (4.13)$$

given that the function $h(q_1, q_2, \ldots q_{d-1})$ is integrable, which means that in the thermodynamic limit $G_s(\vec{R})$ is written as an integral over the single-particle band:

$$G_s(\vec{R}) \approx |S_{+-}|^2 \int_0^{2\pi} \frac{dq_{d-1}}{2\pi} \cdots \int_0^{2\pi} \frac{dq_1}{2\pi} \times \exp[-\hat{\kappa}(\vec{q})|r_\parallel| - i\vec{q}\cdot\vec{r}_\perp] \times \{1 + K_\perp[\hat{\varphi}(\vec{0})S_{++}S_{--}(\Upsilon_1^+ + \Upsilon_1^-) + |S_{+-}|^2(\Upsilon_2^+ + \Upsilon_2^-)\hat{\varphi}(\vec{q})] + O(K_\perp^2)\}. \quad (4.14)$$

If one is interested in correlations in the $\hat{z}$ direction, the asymptotic analysis of (4.14) provides a straightforward formula for the decay of correlation. However, to consider the angular dependence of the correlation function, we need consider decays for which $|r_\parallel|$ and $|r_\perp|$ are comparable. That is, if $\hat{R}\cdot\hat{z} = \cos\theta$, then we are interested in the decay of correlation in directions for which θ is finite. In treating such correlations it is useful to introduce the Fourier-transformed pair correlation function $\hat{G}_s(\vec{q})$. To obtain the decay of $G_s(\vec{R})$ as $\vec{R}$ tends to infinity, by the Abelian and Tauberian theorems of Fourier analysis, we need to treat $\hat{G}_s(\vec{q})$ as $\vec{q}$ tends to zero. The poles of $\hat{G}_s(\vec{q})$ determine the decay of correlation. Thus, in finding the angular dependence of κ, the inverse correlation length, we convert our expansion for $G_s(\vec{R})$ into one for $[\hat{G}_s(\vec{q})]^{-1}$. This is equivalent to summing a certain subset of diagrams in the expansion for $\tilde{M}(\vec{q};0)M(\vec{q},\vec{r}_\perp)$.[26] The problem of determining the angular dependence of the decay of correlation was considered by Onsager[14] who proposed an exact formula for $\kappa(\hat{R})$, which was later derived rigorously by Cheng and Wu.[27] In two dimensions our method reproduces this Onsager-Wu result (we consider this to be a strong confirmation of the general method). In higher dimensions and/or finite fields an analogous result is obtained. For simplicity, however, we shall only present the derivation of $\kappa(\hat{R})$ for the zero-field case, where $\Upsilon_2^+ + \Upsilon_2^- = \cosh(2K_\parallel)$, $S_{++} = S_{--} = 0$, and $S_{+-} = S_{-+} = 1$, so that

$$G_s(\vec{R}) \approx \int_0^{2\pi} \frac{dq_{d-1}}{2\pi} \cdots \int_0^{2\pi} \frac{dq_1}{2\pi} \exp[-\hat{\kappa}(\vec{q})|r_\parallel| - i\vec{q}\cdot\vec{r}_\perp] \times [1 + K_\perp \cosh(2K_\parallel)\hat{\varphi}(\vec{q}) + O(K_\perp^2)] \quad \text{as } |r_\parallel| \to \infty. \quad (4.15)$$

We introduce the Fourier-transformed correlation function

$$\hat{G}_s(\vec{q}) = \sum_{r_\parallel=-\infty}^{\infty} \sum_{\text{all } \vec{r}_\perp} \exp(iq_\parallel r_\parallel + i\vec{q}_\perp\cdot\vec{r}_\perp) G_s(\vec{R}) \quad (\vec{R} = \vec{r}_\perp + r_\parallel\hat{z}). \quad (4.16)$$

Interchanging summation and integration, we easily find that to first order in *both* $K_\perp$ and $K_\parallel$,

$$G_s(q) \approx \frac{1 + K_\perp\hat{\varphi}(\vec{q}_\perp) + O(K_\perp^2)}{1 - 2K_\parallel\cos q_\parallel + O(K_\perp^2)}, \quad (4.17)$$

where we have used $\exp - \hat{\kappa}(\vec{q}_\perp) = 1 + O(K_\perp)$. Since we really want an expansion for $\hat{G}_s(\vec{q}_\perp)^{-1}$, and $K_\perp$ is a small parameter for this problem, we rewrite (4.17) as

$$\hat{G}_s(\vec{q}) \approx [1 - 2K_\parallel\cos q_\parallel - 2K_\perp \sum_{j=1}^{d-1} \cos q_{\perp,j} + O(K^2)]^{-1}. \quad (4.18)$$

We reiterate that (4.17) and (4.18) are valid only for $h = 0$. Equation (4.18) in two dimensions agrees with the exact results found by Onsager,[14] and Cheng and Wu.[27]

Equations (4.14) and (4.18) form the basis for our asymptotic analysis of the decay of spin correlation functions. From (4.14) we obtain the decay of correlation in the layering direction for arbitrary field, and from (4.18) we obtain the angular dependence of the decay in zero field.

We first examine the decay of correlation in the layering direction (assuming, for simplicity, hypercubical layers with nearest-neighbor interactions). The spin correlation becomes

$$G_s(\vec{R}) \approx |S_{+-}|^2 \exp\{-|r_\parallel|[\ln(\mu_+/\mu_-) - \hat{\varphi}(\vec{0})S_{++}(S_{--} - S_{+-})K_\perp + O(K_\perp^2)]\} \times \int_0^{2\pi} \frac{d\theta_1}{2\pi} \cdots \int_0^{2\pi} \frac{d\theta_{d-1}}{2\pi} \Big(\prod_{j=1}^{d-1} \{\cos(r_{\perp j}\theta_j) \exp[|r_\parallel|(2K_\perp|S_{+-}|^2 \times \cos\theta_j + O(K_\perp^2))]\} [1 + K_\perp\hat{\varphi}(\vec{0})S_{++}S_{--}(\Upsilon_1^+ + \Upsilon_1^-) + 2K_\perp|S_{+-}|^2(\Upsilon_2^+ + \Upsilon_2^-) \sum_{j=1}^{d-1} \cos\theta_j + O(K_\perp^2)] \Big). \quad (4.19)$$

It is useful to introduce the following representation for the Bessel function of the first kind with integer order and imaginary argument[28]

$$I_\nu(x) = \int_0^{2\pi} \frac{d\theta}{2\pi} \cos(\nu\theta) e^{x\cos\theta}. \quad (4.20)$$

In terms of Bessel functions the spin correlation function becomes

$$G_s(\vec{R}) = |S_{+-}|^2 e^{-\kappa_0|r_\parallel|}\{H(K_\parallel, K_\perp) \times \prod_{n=1}^{d-1} I_{r_{\perp n}}(\kappa_1|r_\parallel|) + K_\perp|S_{+-}|^2(\Upsilon_2^+ + \Upsilon_2^-) \times \sum_{n=1}^{d-1}[I_{r_{\perp n}-1}(\kappa_1|r_\parallel|) + I_{r_{\perp n}+1}(\kappa_1|r_\parallel|)] \times \prod_{l\neq n} I_{r_{\perp l}}(\kappa_1|r_\parallel|)\}, \quad (4.21)$$

where

$$\kappa_0 = \ln(\mu_+/\mu_-) - \hat{\varphi}(\vec{0})S_{++}(S_{--}+S_{+-})K_\perp + O(K_\perp^2),$$
$$\kappa_1 = 2K_\perp|S_{+-}|^2 + O(K_\perp^2), \quad (4.22)$$
$$H(K_\parallel, K_\perp) = 1 + K_\perp\hat{\varphi}(\vec{0})S_{++}S_{--}(\Upsilon_1^+ + \Upsilon_1^-) + O(K_\perp^2).$$

In our analysis of (4.21) we keep $\vec{r}_\perp$ strictly finite and let $|r_\parallel|$ grow very large. It is easily seen that, to lowest order, $I_{\nu\pm1}(x)$ and $I_\nu(x)$ have the same asymptotic behavior as x tends to infinity. Further, in (5.39), $K_\perp$ is a small parameter. Hence, for our purposes we may as well write

$$G_s(\vec{R}) \approx |S_{+-}|^2 e^{-\kappa_0|r_\parallel|}\prod_{n=1}^{d-1} I_{r_{\perp n}}(\kappa_1|r_\parallel|). \quad (4.23)$$

The net effect of the terms in (4.21) which we have neglected is to generate the first-order angular corrections to the decay along the layering direction. Thus, (4.23) is correct only for $r_{\perp n}=0$ for $n=1, 2, \ldots, d-1$. This restriction to the layering direction is relaxed below in our (less rigorous) calculation of the angular dependence of the decay of correlation.

The Bessel functions in (4.23) may easily be analyzed asymptotically by Laplace's method[28] to find that, as $x\to\infty$,

$$I_0(x) \approx (2\pi x)^{-1/2}e^x[1+\alpha/x+O(x^{-2})], \quad (4.24)$$

where $\alpha=-\frac{1}{4}$, so that the spin correlation function decays as

$$G_s(r_\parallel) \approx |S_{+-}|^2(2\pi)^{-(d-1)/2}e^{-\kappa|r_\parallel|}/(|r_\parallel|)^{(d-1)/2}, \quad (4.25)$$

with κ given (to first order) by $\kappa_0-\kappa_1$, i.e., by (4.4).[1(b)] We have therefore demonstrated the OZ character of the decay of spin correlation in the layering direction of the d-dimensional Ising model in arbitrary magnetic field.

Not surprisingly, the decay of spin correlation in directions other than the layering direction can also be simply expressed in terms of Bessel functions. The Fourier inverse of (4.18) is

$$G_s(\vec{R}) \approx \int_0^{2\pi}\frac{d\theta_0}{2\pi}\cdots\int_0^{2\pi}\frac{d\theta_{d-1}}{2\pi} \times \frac{\exp[-ir_\parallel\theta_0 - i\sum_{n=1}^{d-1}r_{\perp n}\theta_n]}{1-2K_\parallel\cos\theta_0 - 2K_\perp\sum_{n=1}^{d-1}\cos\theta_n + O(K_\perp^2; K_\parallel^2)}. \quad (4.26)$$

Using the integral identity

$$x^{-1} = \int_0^\infty e^{-xs}\,ds \quad (4.27)$$

and interchanging the order of integration, (4.26) is transformed to

$$G_s(\vec{R}) \approx \int_0^\infty ds\, e^{-s} I_{|r_\parallel|}(2K_\parallel s)\prod_{n=1}^{d-1} I_{r_{\perp n}}(2K_\perp s), \quad (4.28)$$

in which the Bessel functions all have large order (since, by assumption $|r_\parallel|\to\infty$ and, further, $|\vec{r}_\perp| = |r_\parallel|\tan\theta$). Thus, we shall require the asymptotic form of $I_\nu(x)$ as ν tends to infinity (for all x), which is given by[28]

$$I_\nu(x) \approx [4\pi^2(\nu^2+x^2)]^{-1/4}\exp[(\nu^2+x^2)^{1/2} - \nu\sinh^{-1}(\nu/x)]. \quad (4.29)$$

With (4.29) at hand we analyze (4.28) using the saddlepoint method.[28] The saddlepoint of the integral S_0 is determined by the so-called saddlepoint condition and is given by

$$S_0 = (r_\parallel^2 + 4K_\parallel^2 S_0^2)^{1/2} + \sum_{l=1}^{d-1}(r_{\perp l}^2 + 4K_\perp^2 S_0^2)^{1/2}. \quad (4.30)$$

Let us introduce a vector $\vec{\kappa}$ with components $\vec{\kappa}_\parallel$, $\vec{\kappa}_{\perp 1}, \ldots, \vec{\kappa}_{\perp d-1}$ defined by

$$r_\parallel = 2K_\perp S_0\sinh\kappa_\parallel, \quad r_{\perp 1} = 2K_\perp S_0\sinh\kappa_{\perp 1}, \ldots, \quad r_{\perp d-1} = 2K_\perp S_0\sinh\kappa_{\perp d-1}, \quad (4.31)$$

which allows us to rewrite the saddlepoint condition as

$$1 = 2K_\perp\sum_{n=1}^{d-1}\cosh\kappa_{\perp n} + 2K_\parallel\cosh\kappa_\parallel. \quad (4.32)$$

Using (4.28), (4.29), (4.31), and a Laplace expansion about the saddlepoint, we find, as $|\vec{R}|\to\infty$,

$$G_s(\vec{R}) \approx (2\pi)^{-(d-1)/2}\, e^{-\vec{\kappa}\cdot\vec{R}}(4K_\parallel^2\sinh^2\kappa_\parallel\prod_{n=1}^{d-1} r_{\perp n}\coth\kappa_{\perp n} + r_\parallel\coth\kappa_\parallel\sum_{n=1}^{d-1}4K_\perp^2\sinh^2\kappa_{\perp n}\prod_{l\neq n} r_{\perp l}\coth\kappa_{\perp l})^{-1/2}, \quad (4.33)$$

where

$$\vec{\kappa}\cdot\vec{R} = \kappa|r_\parallel| + \sum_{n=1}^{d-1}\kappa_{\perp n}|r_{\perp n}|.$$

Introducing a hyperspherical coordinate system

$$r_\parallel = R\cos\theta, \quad r_{\perp n} = R\sin\theta\sin\omega_1\cdots\sin\omega_{n-1}\cos\omega_n, \quad n=1, 2, \ldots, d-1, \quad (4.34)$$

$G_s(\vec{R})$ becomes

$$G_s(\vec{R}) \approx \tilde{G}_d(\vec{\kappa}, K_\parallel, K_\perp, \theta, \{\omega_n\})\,(2\pi R)^{-(d-1)/2}\, e^{-\kappa R\cos\theta} \quad \text{as } R\to\infty\ , \tag{4.35}$$

where to lowest order, $\tilde{G}_d$ is given by

$$\tilde{G}_d(\vec{\kappa}, K_\parallel, K_\perp, \theta, \{\omega_n\}) = \Big(4K_\parallel^2 \prod_{n=1}^{d-1} \sin\theta \sin\omega_1 \cdots \cos\omega_n \coth\kappa_{1n} \sinh^2\kappa_{1n} + \cos\theta \coth\kappa_\parallel \sum_{n=1}^{d-1} 4K_\perp^2 \sinh^2\kappa_{1n} \prod_{l\neq n} \sin\theta \times \sin\omega_1 \cdots \cos\omega_l \coth\kappa_{\perp l}\Big)^{-1/2}\ , \tag{4.36}$$

with

$$R^2 = r_\parallel^2 + \sum_{j=1}^{d-1} r_{\perp j}^2, \quad \kappa_\parallel^2 + \sum_{j=1}^{d-1} \kappa_{\perp j}^2 = \kappa^2\ . \tag{4.37}$$

It remains to show that $\vec{\kappa}$ is independent of $\vec{R}$. First, note that

$$\vec{\kappa} = \left[\sinh^{-1}\left(\frac{r_\parallel}{2K_\parallel S_0}\right),\ \sinh^{-1}\left(\frac{r_{\perp 1}}{2K_\perp S_0}\right),\ \ldots,\ \sinh^{-1}\left(\frac{r_{\perp d-1}}{2K_\perp S_0}\right)\right], \tag{4.38}$$

so that if S_0 equals αR with α independent of R, $\vec{\kappa}$ does not depend on R (although it still depends on $\hat{R} = \vec{R}/R$). Assuming $S_0 = \alpha R$, the saddlepoint condition becomes

$$\alpha = [\alpha^2 4K_\parallel^2 + \cos^2\theta]^{1/2} + \sum_{n=1}^{d-1} [\alpha^2 4K_\perp^2 + \sin^2\theta \sin^2\omega_1 \cdots \cos^2\omega_n]^{1/2}, \tag{4.39}$$

which is patently independent of R. Thus, in (4.35) $\vec{\kappa}$ (and hence $\tilde{G}_d$) is independent of R, and we see that the OZ form for the decay of correlation holds for spin correlation in an arbitrary direction at high temperatures. Although we have only treated the zero field case herein, a similar treatment in a finite field also verifies the OZ form for the decay of spin correlation in an arbitrary direction.

In two dimensions and as above zero field with $K_\perp = K_\parallel = K$, we easily write down S_0 explicitly as αR with α given by

$$\alpha = [1 - 16K^2 + \cdots]^{-1/2} \times \{[1 - \tfrac{1}{2}(1 - 16K^2 + \cdots)\cos^2 2\theta]^{1/2}\}^{1/2}\ , \tag{4.40}$$

so that

$$\sinh\kappa_\perp = \frac{\sin\theta}{2K_\parallel \alpha}, \quad \sinh\kappa_\parallel = \frac{\cos\theta}{2K_\parallel \alpha}\ , \tag{4.41}$$

$$\tilde{G}_2(\vec{\kappa}, K, \theta) = [4K^2(\sin\theta \coth\kappa_\perp \sinh^2\kappa_\parallel + \cos\theta \coth\kappa_\parallel \sinh^2\kappa_\perp)]^{1/2}\ . \tag{4.42}$$

Finally, to first order in K,

$$\alpha \approx (1 - \sin\theta\cos\theta)^{1/2}\ . \tag{4.43}$$

This completes our treatment of the bulk spin correlation functions. We have succeeded in showing the decay of spin pair correlation functions to be Ornstein-Zernike both for arbitrary field in the layering direction and for arbitrary direction in the absence of a field. In two dimensions and zero field, our results agree to first order with the exact results of Cheng and Wu[27] and Onsager.[14]

V. DECAY OF ENERGY-DENSITY CORRELATION FUNCTIONS

In this section, we treat pair correlation functions involving more than two spins. We shall concentrate upon three-spin (spin-energy density) and four-spin (energy-density) pair correlation functions. In zero field we are easily able to construct a proof that all correlation functions on a finite lattice involving *odd* numbers of spins are zero. Of course, if the lattice becomes infinite in two or more dimensions, this argument is vitiated; and we then have an ordering temperature below which the up-down symmetry is broken either by boundary conditions (as we have shown in Paper I) or by an infinitesimal field. However, for all temperatures above this ordering temperature, its conclusions remain correct.

We also produce a proof that the transverse (i.e., perpendicular to the layering direction) energy-density correlation functions are determined by the even particle-number levels in a zero field. This proof is valid so long as the perturbation expansion converges (for all T if N is strictly finite). Thus, the asymptotic decay of transverse energy-density correlation functions is specified by the vacuum and the two-particle levels. In a finite field the decay of these correlation functions is again determined by the single-particle band.

Consider first the $(2l+1)$ spin expectation value in zero magnetic field. In zero field, the transfer matrix K may be written

$$\mathrm{K} = 2^N \cosh^N K_\parallel \exp\Big[\ln V_\parallel \sum_{\vec{x}} \mathrm{n}(\vec{x})\Big] \exp\Big\{\tfrac{1}{2}K_\perp \sum_{\vec{x},\vec{\delta}} \varphi(\vec{\delta})\,[\underline{\psi}^\dagger(\vec{x}) + \underline{\psi}(\vec{x})]\,[\underline{\psi}(\vec{x}+\vec{\delta}) + \underline{\psi}^\dagger(\vec{x}+\vec{\delta})]\Big\}\ . \tag{5.1}$$

This operator does not preserve particle number; but it does preserve the parity of the number of the particles. Hence, since the largest eigenvector is gotten by repeated operations involving transitions induced by $\underline{\mathrm{K}} - \underline{\mathrm{K}}_1$ away from the vacuum state $|\Phi\rangle$, we see that $|\lambda_0\rangle$ only contains states of even particle number. Similarly, the first band of eigenvalues below λ_0 will have states gotten by transitions away from single-particle states. Thus, the first band of states involves only odd numbers of particles. In a like way we see that

the $2n$ band involves only states of even particle number and that the $(2n+1)$ band involves only states of odd particle number. From our work in Paper I we know that $\langle \underline{\sigma}^z(1)\cdots\underline{\sigma}^z(2l+1)\rangle$ may be written in terms of the matrix elements of these spins between eigenvectors of the transfer matrix. In particular, consider the expectation with a single spin in each layer. Then the matrix elements are of the form

$$\langle \lambda_0|\underline{\sigma}^z(1)|\lambda_{n_1},\bar{l}_1\rangle\langle\lambda_{n_1},\bar{l}_1|\underline{\sigma}^z(2)|\lambda_{n_2},\bar{l}_2\rangle\cdots \langle\lambda_{n_{2l}},\bar{l}_{2l}|\underline{\sigma}^z(2l+1)|\lambda_0\rangle\,, \quad (5.2)$$

where in $\{|\lambda_{n_p},\bar{l}_p\rangle\}$, n_p labels the number of particles in the zeroth-order state and $\bar{l}_p$ in an index labelling the states within the band. Now, $\underline{\sigma}^z(\vec{r}) = \underline{\psi}(\vec{r})+\underline{\psi}^\dagger(\vec{r})$ changes the particle number by ± 1. Thus, it takes even-particle-number states into odd-particle-number states and vice versa. Then in (5.2), n_1 must be odd, n_2 even, $\cdots, n_{2l}$ even, for a nonzero matrix element by orthonormality. However, $\langle\lambda_{n_{2l}},\bar{l}_{2l}|\underline{\sigma}^z(2l+1)|\lambda_0\rangle$ is then zero by orthonormality. It is easily seen that putting two or several spins in one or more layers leaves this over-all situation unchanged. This constitutes a proof within the context of the transfer matrix that $\langle\underline{\sigma}^z(1)\cdots\underline{\sigma}^z(2l+1)\rangle = 0$ in zero field.

We now consider the energy-density correlation function. In zero field the Ising Hamiltonian is written

$$-\beta\mathcal{H} = K_\parallel\sum_{r_\parallel}\sum_{\vec{r}_\perp}\underline{\sigma}^z(\vec{r}_\perp,r_\parallel)\underline{\sigma}^z(\vec{r}_\perp,r_\parallel+1) + \tfrac{1}{2}K_\perp\sum_{r_\parallel}\sum_{\vec{r}_\perp}\sum_{\vec{\delta}}\varphi(\vec{\delta})\underline{\sigma}^z(\vec{r}_\perp,r_\parallel)\underline{\sigma}^z(\vec{r}_\perp+\vec{\delta},r_\parallel)\,. \quad (5.3)$$

Thus, we are led to define an energy density

$$\epsilon(\vec{r}_\perp,r_\parallel) = \epsilon_\perp(\vec{r}_\perp,r_\parallel)+\epsilon_\parallel(\vec{r}_\perp,r_\parallel)\,, \quad (5.4)$$

with

$$-\beta\epsilon_\perp(\vec{r}_\perp,r_\parallel) = \tfrac{1}{2}K_\perp\textstyle\sum_{\vec{\delta}}\varphi(\vec{\delta})\underline{\sigma}^z(\vec{r}_\perp,r_\parallel)\underline{\sigma}^z(\vec{r}_\perp+\vec{\delta},r_\parallel)\,, \quad (5.5)$$

$$-\beta\epsilon_\parallel(\vec{r}_\perp,r_\parallel) = K_\parallel\underline{\sigma}^z(\vec{r}_\perp,r_\parallel)\underline{\sigma}^z(\vec{r}_\perp,r_\parallel+1)\,. \quad (5.6)$$

In a finite field this is called the exchange-energy density (or the enthalpy density). We call $\epsilon_\parallel$ the longitudinal energy density, and $\epsilon_\perp$ the transverse energy density.

Of principal interest is the decay of the correlation function $G_{\epsilon_\perp}(\vec{R}) = \langle\delta\epsilon_\perp(\vec{0},0)\,\delta\epsilon_\perp(\vec{r}_\perp,r_\parallel)\rangle$. As $|r_\parallel|$ tends to infinity,

$$G_{\epsilon_\perp}(\vec{R}) \approx \sum_{\vec{q}}[\lambda_1(\vec{q})/\lambda_0]^{|r_\parallel|}\langle\lambda_0|\epsilon_\perp(\vec{0})|\lambda_1(\vec{q})\rangle \times\langle\lambda_1(\vec{q})|\epsilon_\perp(\vec{0})|\lambda_0\rangle + \sum_{\vec{q}_1,\vec{q}_2}[\lambda_2(\vec{q}_1,\vec{q}_2)/\lambda_0]^{|r_\parallel|} \times\langle\lambda_0|\epsilon_\perp(\vec{0})|\lambda_2(\vec{q}_1,\vec{q}_2)\rangle\langle\lambda_2(\vec{q}_1,\vec{q}_2)|\epsilon_\perp(\vec{0})|\lambda_0\rangle\,. \quad (5.7)$$

Now as we have shown above, in zero field, $|\lambda_0\rangle$ consists entirely of states of even particle number and $|\lambda_1(\vec{q})\rangle$ states of odd particle number. The energy density is a two-spin function and , as such, preserves particle number or changes it by 2. This means that $\epsilon_\perp$ cannot connect $|\lambda_0\rangle$ and $|\lambda_1(q)\rangle$ in zero field:

$$\langle\lambda_0|\epsilon_\perp(\vec{0})|\lambda_1(\vec{q})\rangle = \langle\lambda_1(\vec{q})|\epsilon_\perp(\vec{0})|\lambda_0\rangle = 0 \quad (h=0)\,. \quad (5.8)$$

So, in zero field, (5.7) becomes

$$G_{\epsilon_\perp}(\vec{R}) \approx \sum_{\vec{q}_1,\vec{q}_2}[\lambda_2(\vec{q}_1,\vec{q}_2)/\lambda_0]^{|r_\parallel|}\langle\lambda_0|\epsilon_\perp(\vec{0})|\lambda_2(\vec{q}_1,\vec{q}_2)\rangle \times\langle\lambda_2(\vec{q}_1,\vec{q}_2)|\epsilon_\perp(\vec{0})|\lambda_0\rangle\,. \quad (5.9)$$

We developed perturbation-theoretic formulas for λ_0 and $\lambda_2(\vec{q}_1,\vec{q}_2)$; we now employ them to find (when $h=0$)

$$\hat{\kappa}(\vec{q}_1,\vec{q}_2) = \ln[\lambda_0/\lambda_2(\vec{q}_1,\vec{q}_2)] = 2\ln(\coth K_\parallel) - K_\perp[\hat{\varphi}(\vec{q}_1)+\hat{\varphi}(\vec{q}_2)]+O(K_\perp^2)\,. \quad (5.10)$$

We recognize that (5.10) implies

$$\hat{\kappa}(\vec{q}_1,\vec{q}_2) = \hat{\kappa}(\vec{q}_1)+\hat{\kappa}(\vec{q}_2)\,, \quad (5.11)$$

with $\hat{\kappa}(\vec{q})$ defined by (4.4) with $h=0$. It remains to calculate the matrix elements in (5.9) (we set $\vec{r}=0$ and specialize to correlation in the layering directions). The eigenstates $|\lambda_0\rangle$ and $\langle\lambda_0|$ are given by (3.10b) and (3.10c), while $|\lambda_2(q_1,q_2)\rangle$ is given by (3.27) and (3.29). Thus, we have

$$\langle\lambda_0|\epsilon_\perp(\vec{0})|\lambda_2(\vec{q}_1,\vec{q}_2)\rangle = -\tfrac{1}{2}J_\perp\textstyle\sum_{\vec{\delta}}\varphi(\vec{\delta})[\Psi_{\vec{q}_1,\vec{q}_2}(\vec{0},\vec{\delta}) + \Psi_{\vec{q}_1,\vec{q}_2}(\vec{\delta},\vec{0})]+O(K_\perp)\,. \quad (5.12)$$

Similarly, we have

$$\langle\lambda_2(\vec{q}_1,\vec{q}_2)|\epsilon_\perp(\vec{0})|\lambda_0\rangle = -\tfrac{1}{2}J_\perp\textstyle\sum_{\vec{\delta}}\varphi(\vec{\delta})[\Psi^*_{\vec{q}_1,\vec{q}_2}(\vec{0},\vec{\delta}) + \Psi^*_{\vec{q}_1,\vec{q}_2}(\vec{\delta},\vec{0})]+O(K_\perp)\,. \quad (5.13)$$

Hence, for nearest-neighbor interactions upon a hypercubical lattice, we have

$$\langle\lambda_0|\epsilon_\perp(\vec{0})|\lambda_2(\vec{q}_1,\vec{q}_2)\rangle\langle\lambda_2(\vec{q}_1,\vec{q}_2)|\epsilon_\perp(\vec{0})|\lambda_0\rangle = \frac{8J_\perp^2}{N^2}\sum_{l=1}^{d-1}\sum_{n=1}^{d-1}\exp[i(Q_n-Q_l)/2]\sin q_l\sin q_n\,, \quad (5.14)$$

where Q_j and q_j are the $(d-1)$ components of $\vec{Q}=\vec{q}_1+\vec{q}_2$ and $\vec{q}=\tfrac{1}{2}(\vec{q}_2-\vec{q}_1)$, respectively. Because of the translational invariance of the lattice, we may replace the summation in (5.97) over $\vec{q}_1$ and $\vec{q}_2$ by sums over $\vec{Q}$ and $\vec{q}$—the sums running over a Brillouin zone for $\vec{Q}$ and a slightly modified zone for $\vec{q}$.[29] The modification is introduced to avoid double counting a few states near the Brillouin

zone edge and disappears as $\{N_j \to \infty\}$, in which limit, from (5.9), (5.10), and (5.14) we have

$$G_{\epsilon_\perp}(\vec{R}) \approx 8J_1^2 \sum_{l=1}^{d-1}\sum_{n=1}^{d-1} \int_{-\pi}^{\pi} \frac{dq_1}{2\pi} \cdots \int_{-\pi}^{\pi} \frac{dQ_{d-1}}{2\pi} \times e^{i(Q_n - Q_l)/2}\, e^{i|r_\parallel| \hat{\kappa}(\vec{Q},\vec{q})} \sin q_l \sin q_n . \quad (5.15)$$

From parity considerations only the terms with $n = l$ in (5.15) are nonzero; and using the trigonometric identities $\sin^2 x = \frac{1}{2}[1 - \cos 2x]$ and $\cos(x+y) + \cos(x-y) = 2\cos x \cos y$, we find

$$G_{\epsilon_\perp}(\vec{R}) \approx 4(d-1) J_1^2 \exp[-2\ln(\coth K_\parallel)|r_\parallel|] \times \left(\int_{-\pi}^{\pi} \frac{dQ}{2\pi} \int_{-\pi}^{\pi} \frac{dq}{2\pi} e^{4K_\perp |r_\parallel| \cos q} \right)^{d-2} \times \int_{-\pi}^{\pi} \frac{dQ}{2\pi} \int_{-\pi}^{\pi} \frac{dq}{2\pi} (1 - \cos 2q) \times \exp[4K_\perp |r_\parallel| \cos(\tfrac{1}{2}Q) \cos q] \quad \text{as } |r_\parallel| \to \infty . \quad (5.16)$$

Again, as for $G_s(\vec{R})$, we may rewrite (5.16) in terms of $I_\nu(x)$ Bessel functions and asymptotically estimate (5.16) as $|r_\parallel| \to \infty$.[30] The result of the asymptotic analysis is

$$G_{\epsilon_\perp}(\vec{R}) \approx \frac{64\pi \hat{\varphi}(\vec{0}) J_1^2}{(16\pi K_\perp R)^d} e^{-2\kappa R}, \quad (5.17)$$

with κ given by (4.4), with $\vec{q} = 0$. (The details of the analysis are given in the Appendix.) Note that this form reproduces the Hecht-Stephenson result[13] in two dimensions and *generally* disagrees with the OZ prediction. Equation (5.17) is in agreement with the exact two-dimensional results of Stephenson [9] and of Hecht.[9] As discussed in Ref. 1(b), our results differ strikingly from those obtained by Polyakov[31] using diagrammatic techniques. We have shown that in zero field the decay of energy-density correlations is non-OZ simply because the leading asymptotic forms arise out of the two-particle band rather than the single-particle band.

Our result (5.17) is subject to the criticism that it seems to depend crucially on having two spins in the same layer so that the two-particle states enter, and hence $G_{\epsilon_\parallel}(R)$, which has only one spin per layer, might have a different asymptotic form. Actually, this is not the case. It is easily seen that as $K_\perp \to 0$ in zero field (with $\vec{R} = r_\parallel \hat{z}$)

$$G_{\epsilon_\parallel}(R) \approx \sum_{\vec{k},\vec{p}} \sum_{\vec{q}_1,\vec{q}_2} e^{-[\hat{\kappa}(\vec{p}) + \hat{\kappa}(\vec{k})]} e^{-R\hat{\kappa}(\vec{q}_1,\vec{q}_2)} \times \langle \Phi | \sigma^z(\vec{0}) | \vec{k} \rangle \langle \vec{k} | \sigma^z(\vec{0}) | \Psi(\vec{q}_1,\vec{q}_2) \rangle \times \langle \Psi(\vec{q}_1,\vec{q}_2) | \sigma^z(\vec{0}) | \vec{p} \rangle \langle \vec{p} | \sigma^z(\vec{0}) | \Phi \rangle , \quad (5.18)$$

where $|\vec{k}\rangle$ and $|\vec{p}\rangle$ are single-particle running-wave states as in (3.16), and $|\Psi(\vec{q}_1,\vec{q}_2)\rangle$ are the two-particle states defined by (3.27) with (3.29). The simplest way to analyze (5.18) is to use (3.27), perform the direct-space summations—thereby reducing the sums over $\vec{q}_1$ and $\vec{q}_2$ to sums over the product $(\delta_{\vec{q}_1,\vec{k}} - \delta_{\vec{q}_2,\vec{k}})(\delta_{\vec{q}_1,\vec{p}} - \delta_{\vec{q}_2,\vec{p}})$, after which the sums over $\vec{k}$ and $\vec{p}$ are converted to integrals which are then expressed in terms $I_\nu(x)$ for large x, and easily analyzed. The result is identical to (5.17).

The point is that for correlations involving two local operators of the form

$$\underline{A}(r_\parallel^0, \vec{r}_\perp^{\,0}) = \sum_{l=1}^{2n} \sum_{r_{\parallel l}} \sum_{r_{\perp l}} \tilde{A}(\{r_\parallel^0 - r_{\parallel l}\}, \{|\vec{r}_\perp^{\,0} - \vec{r}_{\perp l}|\}) \times \underline{\sigma}^z(\vec{r}_{\perp 1}, r_{\parallel 1}) \cdots \underline{\sigma}^z(\vec{r}_{\perp 2n}, r_{\parallel 2n}) , \quad (5.19)$$

with $\tilde{A}$ a short-ranged kernel, the asymptotic decay of correlation will have its major R dependence determined by the two-particle eigenstates as in (5.9) *and in* (5.18). For example, we are able to generalize (5.17) to the zero-field decay of any correlation function an even number of spins in layer l and an even number of spins in layer $l+R$. For such correlations, then, we have

$$G_{\text{even}}(\vec{R}) \sim R^{-d} e^{-2\kappa R} \quad (R \to \infty), \quad (5.20)$$

because the decay is necessarily determined by the two-particle band. On the other hand, in zero field it is also clear that the decay of correlation functions involving $2n+1$ spins in layer l and $2m+1$ spins in layer $l+R$ is OZ-like. That is,

$$G_{\text{odd}}(\vec{R}) \sim R^{-(d-1)/2} e^{-\kappa R} \quad (R \to \infty) , \quad (5.21)$$

since in this case the decay of correlation is determined by the single-particle band.

We now complete our treatment of the decay of correlation at high temperatures by calculating the asymptotic decay of spin-energy density pair correlation functions and energy density pair correlation functions in a finite field. We shall find that they exhibit the normal OZ-decay.

In finite magnetic field the single-particle contribution to (5.7) does not vanish. The calculation of the single-particle matrix elements being straightforward, we only present the results:

$$G_{\epsilon_\perp}(\vec{R}) \approx S_{++}^2 |S_{+-}|^2 \frac{2\hat{\varphi}(\vec{0})[\hat{\varphi}(\vec{0}) + 1] e^{-\kappa R}}{(4\pi K_\perp |S_{+-}|^2 R)^{(d-1)/2}} , \quad (5.22)$$

$$\langle \delta\epsilon_\perp(\vec{0}, 0)\, \delta S^z(\vec{0}, r_\parallel) \rangle = G_{\epsilon_\perp - s}(\vec{R}) \approx \frac{2\hat{\varphi}(\vec{0}) S_{++} |S_{+-}|^2 e^{-\kappa R}}{(4\pi K_\perp |S_{+-}|^2 R)^{(d-1)/2}} \quad \text{as } R \to \infty . \quad (5.23)$$

Thus, both are OZ with κ defined by (4.4) and $\vec{q}$ equal to zero. Again we can safely generalize our results to say that in finite field any *pair* correla-

tion function will be OZ-like in form because the leading contribution arises from the single-particle band. This is because the matrix elements between the zero-particle and single-particle states are manifestly finite:

$$\langle \Phi | \sigma^z(\vec{x}_1) \cdots \sigma^z(\vec{x}_n) | \vec{q} \rangle = \sum_{j=1}^{n} e^{i\vec{q}\cdot\vec{x}_j} S_{++}^{n-1} S_{+-} \ . \quad (5.24)$$

In a small, but finite, field the two-particle contribution to an arbitrary correlation function retains the form [Eq. (5.20)], so that generally we may expect (1.10) to hold.

VI. SUMMARY

In this work we have considered the asymptotic decay of pair correlation functions in the Ising model at high temperatures and have found that the decay of bulk spin correlation functions is in accord with the OZ prediction for arbitrary magnetic field. Further, in zero field we have considered the angular dependence of the decay of such correlations—finding results which are a direct generalization of the exact two-dimensional result of Onsager[14] and of Cheng and Wu.[27]

On the other hand, the energy-density correlation functions were found to obey the OZ prediction only in nonzero field. In zero field they are found to exhibit the non-OZ form (5.17)—a generalization of exact two-dimensional results of Stephenson[13] and of Hecht.[13] On the other hand, our results are in disagreement with those of Polyakov,[31] as we have discussed previously.

Correlation functions involving an odd number of spins were found to be identically zero in zero field and OZ-like in finite field. Finally, we found that correlations involving a group of $2n$ spins in one layer and a group of $2m$ spins in a distant layer would have the non-OZ behavior typified by the energy-density correlation functions in zero field, while correlations involving $2m+1$ spins in one layer and $2n+1$ spins in a distant layer verify the OZ form in zero field.

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APPENDIX

We derive (5.17) from

$$G_{\epsilon_\perp}(\vec{R}) \approx 4(d-1)J_\perp^2 \exp[-2\ln(\coth K_\parallel)|r_\parallel|] \times \left(\int_{-\pi}^{\pi}\frac{dQ}{2\pi}\int_{-\pi}^{\pi}\frac{dq}{2\pi}\, e^{4K_\perp|r_\parallel|\cos q}\right)^{d-2} \times \int_{-\pi}^{\pi}\frac{dQ}{2\pi}\int_{-\pi}^{\pi}\frac{dq}{2\pi}\,(1-\cos 2q) \times \exp[4K_\perp|r_\parallel|\cos(\tfrac{1}{2}Q)\cos q] \ \text{as} \ |r_\parallel| \to \infty \ . \quad (A1)$$

The integrals in (A1) are analyzed as follows:

$$\int_{-\pi}^{\pi}\frac{dQ}{2\pi}\int_{-\pi}^{\pi}\frac{dq}{2\pi}\exp(4K_\perp|r_\parallel|\cos\tfrac{1}{2}Q\cos q) = \int_{-\pi}^{\pi}\frac{dQ}{2\pi} I_0(4K_\perp|r_\parallel|\cos\tfrac{1}{2}Q) \approx \int_{-\pi}^{\pi}\frac{dQ}{2\pi}(8\pi K_\perp|r_\parallel|\cos\tfrac{1}{2}Q)^{-1/2}\exp(4K_\perp|r_\parallel|\cos\tfrac{1}{2}Q), \quad (A2)$$

$$\int_{-\pi}^{\pi}\frac{dQ}{2\pi}\int_{-\pi}^{\pi}\frac{dq}{2\pi}(1-\cos 2q) \times \exp(4K_\perp|r_\parallel|\cos\tfrac{1}{2}Q\cos q) = \int_{-\pi}^{\pi}\frac{dQ}{2\pi}[I_0(4K_\perp|r_\parallel|\cos\tfrac{1}{2}Q) - I_2(4K_\perp|r_\parallel|\cos\tfrac{1}{2}Q)] \approx \int_{-\pi}^{\pi}\frac{dQ}{2\pi}(8\pi K_\perp|r_\parallel|\cos\tfrac{1}{2}Q)^{-1/2} \times \frac{\exp(4K_\perp|r_\parallel|\cos\frac{1}{2}Q)}{2K_\perp|r_\parallel|\cos\frac{1}{2}Q}, \quad (A3)$$

where we have used the asymptotic form of $I_\nu(z)$ as $|z|$ tends to infinity.[28]

The asymptotic behavior of (A2) and (A3) for large $|r_\parallel|$ is easily extracted using Laplace's method.[28] In both cases the saddlepoint is at the origin and we may replace $\cos\frac{1}{2}Q$ as the denominators of both integrands by unity. In the first case, we obtain

$$\int_{-\pi}^{\pi}\frac{dQ}{2\pi}(8\pi K_\perp|r_\parallel|\cos\tfrac{1}{2}Q)^{-1/2}\exp(4K_\perp|r_\parallel|\cos\tfrac{1}{2}Q) \approx \frac{e^{4K_\perp|r_\parallel|}}{16\pi K_\perp|r_\parallel|}, \quad (A4)$$

and in the second

$$\int_{-\pi}^{\pi}\frac{dQ}{2\pi}(8\pi K_\perp|r_\parallel|\cos\tfrac{1}{2}Q)^{-1/2}\frac{\exp(4K_\perp|r_\parallel|\cos\frac{1}{2}Q)}{2K_\perp|r_\parallel|\cos\frac{1}{2}Q} \approx \frac{e^{4K_\perp|r_\parallel|}}{32\pi K_\perp^2|r_\parallel|^2}. \quad (A5)$$

Hence we obtain the desired result

$$G_\epsilon(\vec{R}) = \frac{64\pi\hat{\varphi}(\vec{0})J_\perp^2}{(16\pi K_\perp R)^d}\, e^{-2\kappa R}, \quad (A6)$$

where $\hat{\varphi}(0) = d-1$, the layer coordination number.

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$$e^{-R/\lambda_1} < |G_s(\vec{R})| < e^{-R/\lambda_2}.$$

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Effects of the Spin-Flop Transition on the Two-Magnon Absorption in MnF_2†

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The effect of the spin-flop transition on the magnon dispersion relations in uniaxial antiferromagnets has been investigated. The contribution of the dipole-dipole interaction is studied in detail for Brillouin-zone-edge magnons. It is shown that the magnon-pair modes shift at the spin-flop transition to lower energies by an amount that is directly related to the $\vec{k}$-dependent contribution of the dipole-dipole interaction. Shifts of the far-infrared two-magnon absorptions in MnF_2 of 0.8 ± 0.2 and 2.15 ± 0.3 cm^{-1} were measured for $\vec{E} \parallel \vec{c}$ and $\vec{E} \perp \vec{c}$, respectively, by Fourier-transform spectroscopy at $T \approx 1.4$ K. These shifts are in agreement with the calculated values and constitute a direct observation of the $\vec{k}$-dependent dipolar energy.

I. INTRODUCTION

MnF_2, as well as many other magnetic insulators, orders antiferromagnetically below its Néel temperature. The elementary spin excitations in such an ordered state, known as spin waves or magnons, have been directly observed in these systems. Observation of single modes (one mag-