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Decay of Order in Classical Many-Body Systems. III. Ising Model at Low Temperature^{*}

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In this work the decay of correlation in the *d*-dimensional Ising model is studied at low temperatures as a function of dimensionality of the lattice and magnetic field *h*. Except for the special case of the two-dimensional zero-field nearest-neighbor lattices, the decay of correlation verifies the Ornstein-Zernike prediction $G_{AB}(\vec{R}) \approx D_{AB}(d, h)R^{-(d-1)/2}e^{-\kappa R}$. For the two-dimensional zero-field case, the Ornstein-Zernike form is replaced by the "anomalous" form $G_{AB}(\vec{R}) \approx D_{AB}R^{-2}e^{-\kappa R}$. This "anomalous" result is shown to arise from the peculiarities of the spectrum of the transfer matrix in this case and is replaced by the Ornstein-Zernike result when further-neighbor forces are present. The results presented herein agree with the previously obtained exact results for the zero-field two-dimensional Ising model.

I. INTRODUCTION

In the first two papers of this series^{1,2} (hereafter referred to as I and II, respectively) the transfer-matrix approach to classical statistical mechanics was developed in a general framework¹ and applied to a study of the decay of pair correlation functions in the *d*-dimensional Ising model at high temperatures.² It was found that an arbitrary pair correlation function defined on the system decays as

$$\begin{aligned} G_{LQ}(\vec{\mathbf{R}}) &\equiv \langle \delta \underline{\mathbf{L}} (\vec{\mathbf{r}}) \delta \underline{\mathbf{Q}} (\vec{\mathbf{r}} + \vec{\mathbf{R}}) \rangle \\ &\approx (A_0 + A_1 R^{-1} + \cdots) R^{-(d-1)/2} e^{-\kappa R} \\ &+ (B_0 + B_1 R^{-1} + \cdots) R^{-d} e^{-2\kappa R} + \cdots, \quad (1.1) \end{aligned}$$

where A_n and B_n factor as $C_n(\underline{\mathbf{L}})C_n(\underline{\mathbf{Q}})$ and $D_n(\underline{\mathbf{L}})D_n(\underline{\mathbf{Q}})$, respectively. If $\underline{\mathbf{L}}$ is an operator composed of an *odd* number of closely spaced spins, the coefficients $C_n(\underline{\mathbf{L}})$ tend to a finite limit as the magnetic field htends to zero, while the coefficients $D_n(\underline{\mathbf{L}})$ tend to zero. On the other hand, if $\underline{\mathbf{L}}$ is composed of an *even* number of such spins, the coefficients $D_n(\underline{\mathbf{L}})$ tend to zero as h tends to zero.² The first series of terms corresponds to the Ornstein-Zernike (OZ) result, while the second series is the leading correction to it. In this paper the analysis of such correlation functions is extended to the *d*-dimensional Ising model at low temperatures. This problem is both more interesting and more difficult than the hightemperature analysis—more interesting because one is able to treat the spontaneously ordered system, more difficult because of the increased complexity of the transfer-matrix spectrum at low temperatures. Indeed, a major impetus for this work was the interest in understanding the "anomalous" decay of correlation in the two-dimensional model below the critical point.³ That is, whereas at high temperatures the spin-pair correlation function $G_s(\vec{\mathbf{R}})$ decays as

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$$G_{\rm s}(\vec{\rm R}) \sim R^{-1/2} e^{-\kappa R}$$
, (1.2)

in agreement with the OZ hypothesis, 2,4 at low temperatures it is found that 3,4

$$G_{\rm s}(\vec{\rm R}) \sim R^{-2} e^{-\kappa R} \quad , \tag{1.3}$$

which does not verify the OZ prediction. However, (1.3) has the form of the first-correction term to the OZ result in (1.1) if 2κ is replaced by κ . The OZ term in (1.1) arises from the single-particle band of the transfer-matrix spectrum,² and the second term arises from the two-particle band.² Thus, one is tempted to speculate that (1.3) reflects the absence of effects due to single4)

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particle states and the dominance of two-particle effects in the spectrum of the two-dimensional zero-field low-temperature transfer matrix. Indeed, it is shown herein that this conjecture is a correct one. The two-dimensional low-temperature zero-field Ising model with nearest-neighbor interactions stands alone in the respect that the eigenstates of its transfer matrix are all states with an even number of particles.³ This anomalous behavior of the low-temperature two-dimensional Ising model has led to speculation^{3(b)} that the OZ theory is not adequate for the treatment of ordered systems in which two or more phases can coexist. In this work such worries are dispelled: the anomaly is that the of two-dimensional Ising model, and not a general property of ordered systems.

In general, except for the zero-field two-dimensional case, the decay of correlation at low temperatures verifies the OZ prediction. In addition, the introduction of second- or further-neighbor interactions in the two-dimensional zero-field case restores the OZ decay law. In these cases the decay of correlation takes the form³

$$\begin{split} G_{AB}(\vec{\mathbf{R}}) &\approx \big[C_0(\underline{\mathbf{A}}) C_0(\underline{\mathbf{B}}) + O(R^{-1}) \big] R^{-(d-1)/2} e^{-\kappa R} \\ &+ \big[D_0(\underline{\mathbf{A}}) D_0(\underline{\mathbf{B}}) + O(R^{-1}) \big] R^{-\kappa} e^{-\kappa' R} \end{split}, \end{split}$$
(1.

where $\kappa < \kappa' < 2\kappa$ and $x = \frac{1}{2}(d-1)$. What happens in this case is that not only the leading term but also the first correction term verify the OZ prediction. The leading term exhibits the dominance of the single-particle states of the transfer-matrix spectrum, while the OZ form of the first correction arises because the nearest-neighbor two-particle states form a band which lies above the bulk of the two-particle band of the transfer matrix. These bound pairs of particles have an obvious "singleparticle" character as evidenced by (1.4).

The duality relations⁵ for the square Ising net are rederived herein from considerations of the form of the transfer matrix. The fact that the decay of energy-density correlation functions at high temperatures in this model is given by the same form (1.3) as the decay of spin correlation functions at low temperatures is seen to be a consequence of the duality relations.

The outline of this work is as follows. Section II is a derivation of the spectrum of the low-temperature Ising transfer matrix. In Sec. II B the transfer matrix is derived in a form suitable for low-temperature perturbation theory. Subsections II C-II E then present the transfer-matrix spectra for the finite-field case, the zero-field case with d > 2, and the zero-field two-dimensional case, respectively. In Sec. III the results of Sec. II are employed to obtain the decay of correlation in the various situations treated. Section IV then

presents a summary of the results.

II. TRANSFER MATRIX AND ITS EIGENVALUE SPECTRUM

A. Introduction

In this section the transfer matrix is expressed in a form suitable for low-temperature perturbation theory. The notation developed in papers I and II will be adhered to throughout. The finitefield case is considered first. This case is similar to the high-temperature case in that there is no long-range order and in that the decay of order follows the OZ prediction.

The states of the Ising system at low temperature are classified most readily according to the number of overturned spins in a layer, that is, the totally aligned state, states with 1, 2, 3, ..., n overturned spins. To zeroth order the eigenstates of the transfer matrix will be just these states—the completely aligned state being the state with largest eigenvalue, the single-particle states having next-largest eigenvalue, etc. In a finite field, the field fixes a preferred direction of alignment. However, in zero field the system is invariant under the total spin-reversal operation so that the state with N - n up spins and n down spins is degenerate with the state obtained from it by reversing all the spins of the layer. Thus, in zero field, the appropriate zeroth-order eigenstates are linear combinations of these states.

The zero-field problem has a natural division into two cases: dimension d equal to 2 and d equal to or greater than 3. This is because at sufficiently low temperatures the system behaves like a group of uncoupled layers. Within a two- or moredimensional layer, it will always require more energy to flip two or more spins from the aligned state than it requires to flip a single spin. This is because the size of the intralayer phase boundary grows as the (d-2)/(d-1) power of the intralayer phase "volume;" hence the total surface tension within a layer, for d equal to or greater than 3, always increases as the phase volume increases. Note, on the other hand, that for d equal to 2, the intralayer phase boundary is a single wrong $(\uparrow - \downarrow$ or -+) bond at either end of the phase. Thus the surface energy is independent of the size of the phase: It requires the same amount of energy to overturn n spins in a row as it does to overturn a single spin. It is shown below that this leads to the result that the first band of eigenvalues below the largest levels is two-particlelike-the two particles being the two crossed bonds at either end of the row of overturned spins. From the results of Paper II, it may be seen that in this fact lies the qualitative explanation of why the low-temperature two-dimensional zero-field spin correlations

decay as $R^{-2}e^{-\kappa R}$ —it is because the asymptotic decay is determined by a two-particle band.

Therefore, in zero field, d equal to 2 and d equal to or greater than 3 are considered separately. In the latter case, of the OZ form for the decay of correlation is regained, although the possibility that for temperatures sufficiently close to T_c , the non-OZ form $R^{-d}e^{-\kappa R}$ is the dominant contribution to the decay of correlation cannot be completely ruled out. However, from the above discussion of the surface energy, it does seem an unlikely possibility.

B. Transfer Matrix at Low Temperatures

There are two very convenient forms for the low-temperature transfer matrix. The first has already been derived in Paper II of this series,² and will be the starting point of the discussion presented herein. The second form is immediately derivable from the first, as shown below.

In Paper II^2 the Ising transfer matrix was shown to have the form

$$\underline{\mathbf{K}} = \left[2\sinh(2K_{\parallel})\right]^{N/2} \exp\left(u_{\parallel}\sum_{\mathbf{r}} \underline{\sigma}^{\mathbf{x}}(\mathbf{\vec{r}})\right) \\ \times \exp\left[\sum_{\mathbf{r}} \left(h\underline{\sigma}^{\mathbf{z}}(\mathbf{\vec{r}}) + \frac{1}{2}K_{\perp}\sum_{\delta} \varphi(\mathbf{\vec{\delta}})\underline{\sigma}^{\mathbf{z}}(\mathbf{\vec{r}})\underline{\sigma}^{\mathbf{z}}(\mathbf{\vec{r}} + \mathbf{\vec{\delta}})\right)\right].$$
(2.1)

In (2.1), $K_{\parallel} = J_{\parallel}/k_BT$, $K_{\perp} = J_{\perp}/k_BT$, $h = gH/k_BT$, and the variable u_{\parallel} is defined by

$$w_{\parallel} = \tanh u_{\parallel} = e^{-2K_{\parallel}}$$

where J_{\parallel} and J_{\perp} are the exchange-coupling energies in the directions parallel and perpendicular to the layering direction, respectively; k_B is Boltzmann's constant, T is the temperature, His the magnetic field, g is the Landé factor, $\varphi(\delta)$ is an interaction shape function, $\sigma^{\mu}(\vec{r})$ is the μ th component of the Pauli spin operator $\vec{\sigma}(\vec{r})$,² and N is the number of sites in a layer. The most straightforward expansion for the matrix K is obtained by noting that u_{\parallel} tends to zero exponentially fast as K_{\parallel} tends to infinity, and hence as $k_BT(=J_{\parallel}/K_{\parallel})$ tends to zero. Thus, at low temperatures it is reasonable to expand the transfer matrix about $u_{\parallel} = 0$. Recall that it was shown in Paper II² that the coupling between layers is provided by the term in (2.1) involving u_{\parallel} ; so with this decomposition of the matrix, the interlayer interactions act at low temperatures as a perturbation on the spectrum of the intralayer matrix.

The transfer matrix may be written in the product form

$$\underline{\mathbf{K}} = \underline{\mathbf{K}}_{1} \underline{\mathbf{K}}_{2} \quad , \tag{2.2}$$

where

$$\underline{\mathbf{K}}_{1} = \exp\left(u_{\parallel} \sum_{\mathbf{\tilde{r}}} \underline{\sigma}^{\mathbf{x}}(\mathbf{\tilde{r}})\right)$$
(2.3)

and

$$K_2 = [2 \sinh(2K_{\parallel})]^{N/2}$$

$$\times \exp\left[\sum_{\vec{\mathbf{r}}} \left(h \underline{\sigma}^{\mathbf{z}}(\vec{\mathbf{r}}) + \frac{1}{2} K_{\perp} \sum_{\vec{\delta}} \varphi(\vec{\delta}) \underline{\sigma}^{\mathbf{z}}(\vec{\mathbf{r}}) \underline{\sigma}^{\mathbf{z}}(\vec{\mathbf{r}} + \vec{\delta}) \right) \right]. \quad (2.4)$$

This is converted to a perturbation-theoretic form by noting that one may write K as

$$\underline{\mathbf{K}} = \underline{\mathbf{K}}_{2} + (\underline{\mathbf{K}}_{1} - \underline{\mathbf{I}})\underline{\mathbf{K}}_{2} = \underline{\mathbf{K}}_{2} + \sum_{n=1}^{\infty} \left[(\underline{\mathbf{K}}_{1} - \underline{\mathbf{I}})\underline{\mathbf{K}}_{2} \right]_{n} , \quad (2.5)$$

with

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$$[(\underline{\mathbf{K}}_1 - \underline{\mathbf{I}})\underline{\mathbf{K}}_2]_n = (1/n!)u_{\parallel}^n \left(\sum_{\vec{\mathbf{r}}} \underline{\sigma}^x(\vec{\mathbf{r}})\right)^n \underline{\mathbf{K}}_2 \quad .$$
(2.6)

These formulas are then a suitable starting point for a study of the low-temperature spectrum. An alternative scheme, which was expounded by Fisher and Camp, ³ is to perform a straightforward expansion on K in powers of $w_{\mu} = \tanh u_{\mu}$.

This scheme takes the following form. The transfer matrix K is written

$$K = K_0 + V$$
 , (2.7)

where \underline{K}_0 contains all those parts of \underline{K} which are diagonal in the $\{\underline{\sigma}^z(\mathbf{\tilde{r}})\}$ representation. That is, if one takes as a basis set the states of a layer labeled by the value $(\mathbf{1} - \mathbf{1})$ of $\underline{\sigma}^z(\mathbf{\tilde{r}})$ for each site $\mathbf{\tilde{r}}$ in the layer, then \underline{K}_0 is diagonal in the representation and \underline{V} is completely off diagonal. The perturbation matrix \underline{V} is then expanded in powers of w_{\parallel} :

$$\underline{\mathbf{V}} = \sum_{n=1}^{\infty} w_{\parallel}^{n} \underline{\mathbf{V}}_{n} \quad . \tag{2.8}$$

This decomposition of \underline{K} leads ultimately to the same physical results as the $\underline{K}_1\underline{K}_2$ decomposition described above. However, it enables a somewhat simpler graph theoretical expansion of \underline{K} . On the other hand, the $\underline{K}_1\underline{K}_2$ expansion leads to a straightforward treatment of the duality of the square Ising net.⁵ Since the $\underline{K}_0 + \underline{V}$ decomposition has already been described by Fisher and Camp,³ the $\underline{K}_1\underline{K}_2$ decomposition will be developed in detail herein.

To simplify the analysis presented below it is useful to reexpress $\sigma^{x}(\vec{\mathbf{r}})$ in terms of $\sigma^{*}(\vec{\mathbf{r}})$, the spin-half raising and lowering operators⁶:

$$\underline{\sigma}^{x}(\mathbf{\vec{r}}) = \underline{\sigma}^{+}(\mathbf{\vec{r}}) + \underline{\sigma}^{-}(\mathbf{\vec{r}}) \quad .$$
 (2.9)

It is easily verified that the spin operators $\underline{\sigma}^{\star}(\mathbf{\tilde{r}})$ obey the same Pauli algebra as the creation and annihilation operators $\underline{\psi}^{\dagger}(\mathbf{\tilde{r}})$ and $\underline{\psi}(\mathbf{\tilde{r}})$ employed for the high-temperature analysis presented in Paper II, ² namely,

$$\underline{\sigma}^{z}(\mathbf{\ddot{r}}) = 2\sigma^{+}(\mathbf{\ddot{r}})\sigma^{-}(\mathbf{\ddot{r}}) - 1 = 1 - 2\sigma^{-}(\mathbf{\ddot{r}})\sigma^{+}(\mathbf{\ddot{r}}) \quad , \qquad (2.10)$$

$$\left[\sigma^{\pm}(\vec{\mathbf{r}}), \sigma^{\pm}(\vec{\mathbf{r}}')\right] = 0 \quad , \tag{2.11}$$

(2.12)

$$\{\sigma^{+}(\vec{\mathbf{r}}), \sigma^{-}(\vec{\mathbf{r}})\} = 1$$
, (2.13)

where [A, B] and $\{A, B\}$ are the commutator and anticommutator of A and B, respectively. If the vacuum state is $|\Phi(+)\rangle$; the state with all spins in the layer in their $(\mathbf{1})$ state, and if particles are taken to be spins in their (i) state, then $\sigma(\vec{r})$ creates a particle on site \vec{r} , while $\sigma^{*}(\vec{r})$ destroys such a particle. In addition, the number operator is then simply given by $\sigma(\vec{r})\sigma(\vec{r}) = \frac{1}{2} [1 - \sigma(\vec{r})].$ Of course if the vacuum is taken to be $|\overline{\Phi}(-)\rangle$, the state with all spins of the layer in their (\mathbf{i}) state, and particles are taken to be (\mathbf{i}) spins, then $\sigma^{*}(\vec{r})$ is the particle creation operator, $\sigma^{-}(\vec{r})$ the destruction operator, and $\sigma^{*}(\vec{r})\sigma^{-}(\vec{r}) = \frac{1}{2} \left[1 + \sigma^{z}(\vec{r})\right]$ the relevant number operator. Throughout Secs. IIC and IID, spin deviations away from the completely ordered states $|\Phi(\pm)\rangle$ will be referred to as type (\pm) particles.

C. Finite-Field Low-Temperature Spectrum

This section presents an analysis of the spectrum of the Ising transfer matrix at low temperature and nonzero magnetic field. For simplicity the detailed analysis is presented for a hypercubical lattice with nearest-neighbor interactions, although the results obtained are easily seen to apply even with further-neighbor forces.

This layering direction is taken, as in Paper I, ¹ to be the \hat{z} direction, which is also taken to be colinear with the magnetic field $\mathbf{h} = h\hat{z}$. Thus, a spin is in its up $[(\mathbf{i})$ or $(+\frac{1}{2})]$ eigenstate of $\underline{\sigma}^{\mathbf{z}}$ when it points in the positive \hat{z} direction, and in its down $[(\mathbf{i})$ or $(-\frac{1}{2})]$ eigenstate when it points along the negative \hat{z} direction. Note that \underline{K}_2 is diagonal in the $\{\underline{\sigma}^{\mathbf{z}}(\mathbf{\hat{r}})\}$ representation, so that its states may be labeled by the number of overturned spins or "particles."

As noted above it is useful to define the two vacuum states $|\Phi(+)\rangle$ and $|\Phi(-)\rangle$, which are the states of \underline{K}_2 with all spins in their (†) and (†) eigenstates, respectively. In nonzero field only the spectrum of type (+) particles is relevant. However, in zero field $|\Phi(+)\rangle$ and $|\Phi(-)\rangle$ will be the two degenerate eigenstates of the largest eigenvalue of \underline{K}_2 .

In contrast with the high-temperature situation² for which the zeroth-order eigenvalues of K depend only on the particle number, here the eigenvalue spectrum depends also on the "connectivity" of the particles. That is, it costs less energy to overturn two neighboring spins than it does two nonneighboring spins—there are two fewer "wrong" bonds in the former case than in the latter—so that the eigenstates of two neighboring particles have larger eigenvalues than those of two separated particles. Thus these two-particle bound states form a subband lying a finite distance above the bulk of the two-particle band. Of course the same considerations apply to the *n*-particle spectra with $n \ge 3$. The spectrum of K_2 in finite field is displayed in Fig. 1. In this figure, $\Lambda_0(\pm)$ is the eigenvalue of $|\Phi(\pm)\rangle$, and the *n*-particle eigenstates are denoted by

$$\left| \vec{\mathbf{r}}_{1}, \vec{\mathbf{r}}_{2}, \ldots, \vec{\mathbf{r}}_{n}(\pm) \right\rangle = \underline{\sigma}^{\dagger}(\vec{\mathbf{r}}_{1}) \underline{\sigma}^{\dagger}(\vec{\mathbf{r}}_{2}) \cdots \underline{\sigma}^{\dagger}(\vec{\mathbf{r}}_{n}) \left| \Phi(\pm) \right\rangle .$$

$$(2.14)$$

If one denotes the *n*-particle eigenvalues by $\Lambda_{n\alpha}(\pm)$, where $\alpha = a$, *b*, *c*, ... orders the eigenvalues at fixed particle number, *n*, then Λ_{2a} is the eigenvalue of two neighboring particles, while Λ_{2b} is that of two separated particles. Similarly Λ_{3a} , Λ_{3b} , and Λ_{3c} are, respectively, the eigenvalues of three connected particles, of an isolated particle together with a bound pair of particles, and of three isolated particles.

It is easily shown that the eigenvalues $\Lambda_{n\alpha}(-)$ with *n* finite are exponentially damped with respect to $\Lambda_{n\alpha}(+)$ as the number of sites, *N*, in a layer tends to infinity. For example, letting

$$t_{\parallel} = [2\sinh(2K_{\parallel})]^{1/2} , \qquad (2.15)$$

the eigenvalues $\Lambda_0(\pm)$, $\Lambda_1(\pm)$, $\Lambda_{2a}(\pm)$, and $\Lambda_{2b}(\pm)$ are written

$$\Lambda_{0}(\pm) = t_{\parallel}^{N} \exp\left[\frac{1}{2}N\hat{\varphi}(0)K_{\perp} \pm Nh\right], \qquad (2.16a)$$

$$\Lambda_1(\pm) = t_{||}^N \exp[\frac{1}{2}(N-4)\hat{\varphi}(\vec{0})K_1 \pm (N-2)h]$$
,

(2.16b)

$$\Lambda_{2a}(\pm) = t_{\parallel}^{N} \exp\left[\frac{1}{2}(N-8)\hat{\varphi}(\vec{0})K_{\perp} + 2K_{\perp} \pm (N-4)h\right] ,$$
(2.16c)

and

$$\Lambda_{2b}(\pm) = t_{\parallel}^{N} \exp\left[\frac{1}{2}(N-8)\hat{\phi}(0)K_{\perp} \pm (N-4)h\right],$$
(2.16d)

where $\hat{\varphi}(\vec{0})$ is the $\vec{q} = \vec{0}$ component of the Fourier transform of the interaction shape function $\varphi(\vec{\delta})$.² Thus, it is seen that

$$\Lambda_{n\alpha}(-)/\Lambda_{n\alpha}(+) = e^{-2(N-n)\hbar}$$
 (2.17)

So, with h > 0, *n* finite, and *N* tending to infinity, $\Lambda_{n\alpha}(-)$ may be ignored with respect to $\Lambda_{n\alpha}(+)$.





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Of course (2.17) implies that for h = 0, $\Lambda_{n\alpha}(-) = \Lambda_{n\alpha}(+)$, and the spectrum of K₂ doubles up.

The spectrum of the full matrix K may be deduced from that of \underline{K}_2 by introducing $(\underline{K}_1 - \underline{I})\underline{K}_2$ as an additive perturbation on \underline{K}_2 . The perturbation formulas have been presented in Paper II,² and will not be repeated herein. Rather, they will be taken over directly and applied to this problem.

In a nonzero magnetic field it turns out that the level shifts are second order in u_{\parallel} since $[(\underline{K_1} - \underline{I})\underline{K_2}]_1$ has no particle number conserving terms so that its matrix elements between states with equal particle number are zero. Thus, second-order perturbation theory for $[(\underline{K_1} - \underline{I})\underline{K_2}]_1$ together with first-order theory for $[(\underline{K_1} - \underline{I})\underline{K_2}]_2$ must be employed in order to correctly obtain the low-order spectrum of K.

1. Largest Eigenvalue

The largest eigenvalue and its eigenvector are found to be

$$\lambda_{0}(+) \approx \Lambda_{0}(+) \{ 1 + \frac{1}{2} N u_{\parallel}^{2} [1 + \Gamma_{1,1}(K_{\perp}, h)] + O(u_{\parallel}^{3}) \}$$
(2.18)

$$|\lambda_0(+)\rangle \approx |\Phi(+)\rangle + u_{||}\Gamma_{1,1}e^{2\hat{\varphi}(\vec{0})K_1+2\hbar} \sum_{\vec{r}} |\vec{r}(+)\rangle + O(u_{||}^2),$$
(2.19)

where $\Gamma_{n,m}(K_{\perp},h)$ is given by

$$\Gamma_{n,m}(K_{\perp},h) = \{ \exp\left[2n\hat{\varphi}(0)K_{\perp} + 2mh\right] - 1 \}^{-1} , \qquad (2.20)$$

and $\Lambda_0(+) = t_{\parallel}^N \exp[\frac{1}{2}N\hat{\varphi}(\mathbf{0})K_1 + N\hbar]$ is the largest eigenvalue of \underline{K}_2 .

2. Single-Particle Levels

The single-particle band is found by breaking the N-fold degeneracy of the single-particle eigenstates of \underline{K}_2 via second-order perturbation theory. It is easily seen that to do so one must diagonalize the second-order Rayleigh-Schrödinger diagrams, ^{2,6} i.e., those diagrams linking a particle on site $\overline{\mathbf{r}}$ with one on site $\overline{\mathbf{r}}'$ via either the vacuum or the two particle states—all other intermediate states being disallowed by particle number conservation.

The matrix to be diagonalized is

$$M^{*}(\vec{\mathbf{r}},\vec{\mathbf{r}}') = \langle \vec{\mathbf{r}}(+) | [(\underline{\mathbf{K}}_{1}-\underline{\mathbf{I}})\underline{\mathbf{K}}_{2}]_{2} | \vec{\mathbf{r}}'(+) \rangle - [\Lambda_{0}(+) - \Lambda_{1}(+)]^{-1} \langle \vec{\mathbf{r}}(+) | [(\underline{\mathbf{K}}_{1}-\underline{\mathbf{I}})\underline{\mathbf{K}}_{2}]_{1} | \Phi(+) \rangle \langle \Phi(+) | [(\underline{\mathbf{K}}_{1}-\underline{\mathbf{I}})\underline{\mathbf{K}}_{2}]_{1} | \vec{\mathbf{r}}'(+) \rangle \\ + \{ [\Lambda_{1}(+) - \Lambda_{2, b}(+)]^{-1} - [\Lambda_{1}(+) - \Lambda_{2, b}(+)]^{-1} \} \sum_{\vec{\mathbf{r}}_{1}} \sum_{\vec{\mathbf{b}}} \langle \vec{\mathbf{r}}(+) | [(\underline{\mathbf{K}}_{1}-\underline{\mathbf{I}})\underline{\mathbf{K}}_{2}]_{1} | \vec{\mathbf{r}}_{1}, \vec{\mathbf{r}}_{1} + \vec{\mathbf{\delta}}(+) \rangle \langle \vec{\mathbf{r}}_{1}, \vec{\mathbf{r}}_{1} + \vec{\mathbf{\delta}}(+) | [(\underline{\mathbf{K}}_{1}-\underline{\mathbf{I}})\underline{\mathbf{K}}_{2}]_{1} | \vec{\mathbf{r}}'(+) \rangle \\ + [\Lambda_{1}(+) - \Lambda_{2, b}(+)]^{-1} \sum_{\vec{\mathbf{r}}_{1}} \sum_{\vec{\mathbf{r}}_{2}} \langle \vec{\mathbf{r}}(+) | [(\underline{\mathbf{K}}_{1}-\underline{\mathbf{I}})\underline{\mathbf{K}}_{2}]_{1} | \vec{\mathbf{r}}_{1}, \vec{\mathbf{r}}_{2}(+) \rangle \langle \vec{\mathbf{r}}_{1}, \vec{\mathbf{r}}_{2}(+) | [(\underline{\mathbf{K}}_{1}-\underline{\mathbf{I}})\underline{\mathbf{K}}_{2}]_{1} | \vec{\mathbf{r}}'(+) \rangle , \quad (2.21)$$

where the summation over $\overline{\delta}$ is restricted to sites which are nearest neighbors of the site \overline{r}_1 . In contrast, the summation over \overline{r}_2 is unrestricted. The matrix elements in (2.21) may be evaluated, yielding

$$M^{\star}(\mathbf{\ddot{r}},\mathbf{\ddot{r}}') = u_{\parallel}^{2} \Lambda_{1}(+) \left(A\delta(\mathbf{\ddot{r}},\mathbf{\ddot{r}}') + B \sum_{\mathbf{\ddot{o}}} \delta(\mathbf{\ddot{r}},\mathbf{\ddot{r}}'+\mathbf{\ddot{o}}) \right),$$
(2.22)

with

$$A = \frac{1}{2} (N-2) + \hat{\varphi}(\vec{0}) (e^{2h - 4K_{\perp} + 2\hat{\varphi}(\vec{0})K_{\perp}} - 1)^{-1} + (N-2 - \hat{\varphi}(\vec{0}))\Gamma_{1,1}(K_{\perp}, h) \quad (2.23)$$

and

$$B = (e^{2h - 4K_{\perp} + 2\hat{\varphi}(\vec{0})K_{\perp}} - 1)^{-1} - \Gamma_{1,1}(K_{\perp}, h) \quad . \qquad (2.24)$$

In (2.22) $\delta(\mathbf{x}, \mathbf{y})$ is the Kronecker δ , equal to 1 if

 $\vec{\mathbf{x}} = \vec{\mathbf{y}}$ and zero otherwise.

The matrix $M^*(\mathbf{\tilde{r}}, \mathbf{\tilde{r}}')$ is diagonalized by a unitary transformation to the basis

$$\left|\vec{\mathbf{q}}(+)\right\rangle = N^{-1/2} \sum_{\vec{\mathbf{r}}} e^{i\vec{\mathbf{q}}\cdot\vec{\mathbf{r}}} \left|\vec{\mathbf{r}}(+)\right\rangle , \qquad (2.25)$$

where the vectors \vec{q} have components given by $q_i = 2\pi n_i/N_i$ and $n_i = 1, 2, \ldots, N_i$ (N_i being the number of sites in the *i*th layer direction, $i = 1, 2, \ldots, d-1$). The single-particle eigenvalues and eigenvectors are then found to be

$$\lambda_{1}[\vec{q}(+)] = \Lambda_{1}(+) \left[1 + u_{\parallel}^{2} \left(A + 2B \sum_{j=1}^{d-1} \cos(q_{j}) \right) + O(u_{\parallel}^{4}) \right]$$
(2. 26)

and

$$\lambda_{1}(\vec{q})(+) = N^{-1/2} \sum_{\vec{r}} e^{i\vec{q}\cdot\vec{r}} \left(\left| \vec{r}(+) \right\rangle - u_{\parallel}\Gamma_{1,1}(K_{\perp},h) \left| \Phi(+) \right\rangle - u_{\parallel} \left[(e^{-2h+4K_{\perp}-2\hat{\varphi}(\vec{0})K_{\perp}} - 1)^{-1} - \Gamma_{-1,-1}(K_{\perp},h) \right] \times \sum_{\vec{r}} \left| \vec{r}, \vec{r} + \vec{\delta}(+) \right\rangle - u_{\parallel}\Gamma_{-1,-1}(K_{\perp},h) \sum_{\vec{r}'} \left| \vec{r}, \vec{r}' \right\rangle + O(u_{\parallel}^{3}) , \quad (2.27)$$

where in (2.27) the $\vec{\mathbf{r}}$ and $\vec{\mathbf{r}}'$ sums extend over all layer sites, while the sum over $\vec{\delta}$ extends only over nearest-neighbor vectors of the layer. As in Paper II, ² since K is not Hermitian, $\langle \lambda_1(\vec{\mathbf{q}})(+) |$ is not given by the Hermitian conjugate of $|\lambda_1(\vec{\mathbf{q}})(+)\rangle$, but rather must be calculated separately. It is obtained by replacing $e^{i\vec{\mathbf{q}}\cdot\vec{\mathbf{r}}}$ by $e^{-i\vec{\mathbf{q}}\cdot\vec{\mathbf{r}}}$, $\Lambda_i/(\Lambda_i - \Lambda_j)$ by $\Lambda_j/(\Lambda_i - \Lambda_j)$, and $|\cdots\rangle$ by $\langle \cdots |$ in $|\lambda_1(\vec{\mathbf{q}})(+)\rangle$. The resulting expression becomes

$$\langle \lambda_{1}(\vec{q})(+) | = N^{-1/2} \sum_{\vec{r}} e^{-i\vec{q} \cdot \vec{r}}$$

$$\times \left(\langle \vec{r}(+) | + u_{\parallel} \Gamma_{-1,-1}(K_{\perp},h) \langle \Phi(+) | + u_{\parallel} \left[(e^{2h - 4K_{\perp} + 2\hat{\psi}(\vec{0})K_{\perp}} - 1)^{-1} - \Gamma_{1,1}(K_{\perp},h) \right] \sum_{\vec{0}} \langle \vec{r}, \vec{r} + \vec{\delta}(+) | + u_{\parallel} \Gamma_{1,1}(K_{\perp},h) \sum_{\vec{r}_{1}} \langle \vec{r}, \vec{r}_{1}(+) | \right) + O(u_{\parallel}^{3}) .$$

$$(2.28)$$

3. Bound-Pair Levels

The leading term in the asymptotic expansion for the decay of correlation may be obtained from the knowledge of the largest level and the singleparticle band.^{1,2} In particular, the inverse range of correlation κ is given by $\kappa = \ln[\lambda_0(+)/|\lambda_1[\vec{q}(+)]|]$, with $\vec{q} = \vec{0}$, as shown in Papers I and II.^{1,2} However, to obtain the next term in the expansion, one must consider the next band of eigenvalues below the single-particle band, namely, the band of states composed of two neighboring particles. As noted above there is a finite gap (due to the smaller number of wrong bonds) between this band and the remainder of the two-particle band. Hence, these states are referred to herein as bound-pair states.

Again the first-order corrections to the eigenvalues are identically zero, and one must diagonalize the second-order diagrams:

$$\begin{split} M^{(*)}(\vec{r},\vec{r}+\vec{\delta};\vec{r}',\vec{r}'+\vec{\delta}') &= \langle \vec{r},\vec{r}+\vec{\delta}(+) \left| \left[(\underline{K}_{1}-\underline{I})\underline{K}_{2} \right]_{2} \left| \vec{r}',\vec{r}'+\vec{\delta}'(+) \rangle \right. \\ &+ \langle \vec{r},\vec{r}+\vec{\delta}(+) \left| \left[(\underline{K}_{1}-\underline{I})\underline{K}_{2} \right]_{1} \right| \Phi(+) \rangle \langle \Phi(+) \right| \left[(\underline{K}_{1}-\underline{I})\underline{K}_{2} \right]_{1} \left| \vec{r}',\vec{r}'+\vec{\delta}'(+) \rangle / \left[\Lambda_{2a}(+) - \Lambda_{0}(+) \right] \right. \\ &+ \sum_{\vec{x}} \langle \vec{r},\vec{r}+\vec{\delta}(+) \right| \left[(\underline{K}_{1}-\underline{I})\underline{K}_{2} \right]_{1} \left| \vec{x}(+) \rangle \langle \vec{x}(+) \left| \left[(\underline{K}_{1}-\underline{I})\underline{K}_{2} \right]_{1} \right| \vec{r}',\vec{r}'+\vec{\delta}' \rangle / \left[\Lambda_{2a}(+) - \Lambda_{1}(+) \right] \right. \\ &+ \sum_{\vec{x}} \sum_{\vec{\gamma}_{1}} \sum_{\vec{\gamma}_{2}} \langle \vec{r},\vec{r}+\vec{\delta}(+) \right| \left[(\underline{K}_{1}-\underline{I})\underline{K}_{2} \right]_{1} \left| \vec{x},\vec{x}+\vec{\gamma}_{1},\vec{x}-\vec{\gamma}_{2}(+) \rangle \\ &\times \langle \vec{x},\vec{x}+\vec{\gamma}_{1},\vec{x}-\vec{\gamma}_{2}(+) \right| \left[(\underline{K}_{1}-\underline{I})\underline{K}_{2} \right]_{1} \left| \vec{r}',\vec{r}'+\vec{\delta}'(+) \rangle / \left[\Lambda_{2a}(+) - \Lambda_{3a}(+) \right] \\ &+ \sum_{\vec{x}} \sum_{\vec{\gamma}} \sum_{\vec{\gamma}} \sum_{\vec{z}} \langle \vec{r},\vec{r}+\vec{\delta}(+) \right| \left[(\underline{K}_{1}-\underline{I})\underline{K}_{2} \right]_{1} \left| \vec{x},\vec{x}+\vec{\gamma},\vec{z}(+) \rangle \langle \vec{x},\vec{x}+\vec{\gamma},\vec{z}(+) \right| \\ &\times \left[(\underline{K}_{1}-\underline{I})\underline{K}_{2} \right]_{1} \left| \vec{r}',\vec{r}'+\vec{\delta}'(+) \rangle / \left[\Lambda_{2a}(+) - \Lambda_{3b}(+) \right] , \quad (2.29) \end{split}$$

where $\overline{\delta}$, $\overline{\delta}'$, $\overline{\gamma}$, $\overline{\gamma}_1$, and $\overline{\gamma}_2$ are nearest-neighbor lattice vectors, and the sum over the vector \overline{z} runs over all lattice sites except \overline{x} , $\overline{x}+\overline{\gamma}$, and their respective nearest-neighbor sites, and double counting of states is explicitly avoided in all sums over intermediate states. It turns out that the diagonalization of this matrix is equivalent to obtaining the equation of motion of a single dimer diffusing throughout a hypercubical lattice of dimension d-1. In particular the eigenstates will again be running waves; but now they will additionally have a polarization quantum number, and the eigenvalue spectrum breaks into several branches labeled by the polarization index.

The second-order matrix is written

$$M^{(+)}(\mathbf{\ddot{r}}, \mathbf{\ddot{r}} + \mathbf{\ddot{\delta}}; \mathbf{\ddot{r}}', \mathbf{\ddot{r}}' + \mathbf{\ddot{\delta}}') = u_{\parallel}^{2} \Lambda_{2a}(+) \left(\left[\delta(\mathbf{\ddot{r}}, \mathbf{\ddot{r}}') + \delta(\mathbf{\ddot{r}}, \mathbf{\ddot{r}}' + \mathbf{\ddot{\delta}}') + \delta(\mathbf{\ddot{r}}', \mathbf{\ddot{r}} + \mathbf{\ddot{\delta}}) + \delta(\mathbf{\ddot{r}} + \mathbf{\ddot{\delta}}, \mathbf{\ddot{r}}' + \mathbf{\ddot{\delta}}') \right] \\ \times \left\{ 1 + \Lambda_{1}(+) / \left[\Lambda_{2a}(+) - \Lambda_{1}(+) \right] + 3\Lambda_{3a}(+) / \left[\Lambda_{2a}(+) - \Lambda_{3a}(+) \right] + \left[N - 2\hat{\varphi}(\mathbf{\ddot{0}}) \right] \Lambda_{3b}(+) / \left[\Lambda_{2a}(+) - \Lambda_{3b}(+) \right] \right\} \\ + 3\Lambda_{3a}(+) / \left[\Lambda_{2a}(+) - \Lambda_{3a}(+) \right] \left[\delta(\mathbf{\ddot{r}}, \mathbf{\ddot{r}}') \delta(\mathbf{\ddot{\delta}}, \mathbf{\ddot{\delta}}') + \delta(\mathbf{\ddot{r}}, \mathbf{\ddot{r}}' + \mathbf{\ddot{\delta}}') \delta(-\mathbf{\ddot{\delta}}, \mathbf{\ddot{\delta}}') \right] \right). \quad (2.30)$$

This matrix is block diagonalized by the runningwave transformation to the matrix

$$\times M^{(+)}(\vec{\mathbf{r}},\vec{\mathbf{r}}+\vec{\delta};\vec{\mathbf{r}}',\vec{\mathbf{r}}'+\vec{\delta}')e^{i\vec{\mathbf{q}}'\cdot\vec{\mathbf{r}}'},\quad(2.31)$$

$$M^{(+)}(\vec{\mathbf{q}}, \vec{\mathbf{q}}'; \vec{\delta}, \vec{\delta}') = (1/N) \sum_{\vec{\mathbf{r}}} \sum_{\vec{\mathbf{r}}'} e^{-i\vec{\mathbf{q}}\cdot\vec{\mathbf{r}}}$$

so that

(2.32)

(2.35)

$$M^{(+)}(\vec{\mathbf{q}},\vec{\mathbf{q}}';\vec{\delta},\vec{\delta}') = \delta(\vec{\mathbf{q}},\vec{\mathbf{q}}')\tilde{M}^{(+)}(\vec{\mathbf{q}};\vec{\delta},\vec{\delta}') ,$$

with

$$\begin{split} \tilde{M}^{(+)}(\vec{\mathfrak{q}}, \vec{\mathfrak{5}}, \vec{\mathfrak{5}}') &= M_1(1 + e^{-i\vec{\mathfrak{q}}\cdot\vec{\mathfrak{5}}'} + e^{i\vec{\mathfrak{q}}\cdot\vec{\mathfrak{5}}} + e^{i\vec{\mathfrak{q}}\cdot(\vec{\mathfrak{5}}-\vec{\mathfrak{5}}')}) \\ &+ M_2 \delta(\vec{\mathfrak{5}}, \vec{\mathfrak{5}}') + M_2 \delta(-\vec{\mathfrak{5}}, \vec{\mathfrak{5}}') e^{2i\vec{\mathfrak{q}}\cdot\vec{\mathfrak{5}}} \end{split}$$

$$(2.33)$$

In (2.33), M_1 and M_2 are given by

$$M_{1} = u_{\parallel}^{2} \Lambda_{2a}(+) \{ 1 + \Lambda_{1}(+) / [\Lambda_{2a}(+) - \Lambda_{1}(+)] \\ + 3\Lambda_{3a}(+) / [\Lambda_{2a}(+) - \Lambda_{3a}(+)] + [N - 2\hat{\varphi}(\vec{0})] \\ \times \Lambda_{3b}(+) / [\Lambda_{2a}(+) - \Lambda_{3b}(+)] \}$$
(2.34)

and

$$M_{2} = 3u_{\parallel}^{2}\Lambda_{2a}(+)\Lambda_{3a}(+)/[\Lambda_{2a}(+) - \Lambda_{3a}(+)]$$

Thus, to obtain the bound-pair spectrum in second order, it suffices to diagonalize the block matrices $M^{(+)}(\mathbf{\bar{q}}; \mathbf{\bar{\delta}}, \mathbf{\bar{\delta}}')$ for each allowed value of $\mathbf{\bar{q}}$. To avoid double counting, one may require that $\overline{\delta}$ and $\overline{\delta}'$ both be greater than zero using the "dictionary" ordering introduced in Paper II.² [Then the term in (2.33) involving $\delta(-\overline{\delta}, \overline{\delta}')$ is identically zero.] Further, it is useful to remove the part of $M^{(+)}(\overline{q}; \overline{\delta}, \overline{\delta}')$, which is proportional to the identity matrix $\delta(\overline{\delta}, \overline{\delta}')$, since this piece of $M^{(+)}(\overline{q}; \overline{\delta}, \overline{\delta}')$ remains diagonal under any unitary transformation.

The diagonalization of (2, 33) depends of course on the lattice involved. For two-dimensional lattice (d=2), the layers are one dimensional, and $M^{(+)}(\bar{q}; \bar{\delta}, \bar{\delta}')$ is trivally found:

$$M^{(+)}(q; 1, 1) = M_1(2 + 2\cos q) + M_2$$

In a three-dimensional simple cubic lattice (d=3), each layer is a square net. Labeling the layer axes by \hat{x} and \hat{y} , the nearest-neighbor vectors are $\tilde{\delta}_1 = \hat{x}$ and $\tilde{\delta}_2 = \hat{y}$. Thus, one has

$$\underline{\mathbf{M}}^{(+)}(\mathbf{\vec{q}}) = (M_2 + 2M_1)\mathbf{\underline{I}} + \begin{bmatrix} 2M_1 \cos(q_x) & M_1(1 + \phi^{-1} + \zeta + \zeta/\phi) \\ M_1(1 + \phi + \zeta^{-1} + \phi/\zeta) & 2M_1 \cos(q_y) \end{bmatrix} , \qquad (2.36)$$

where $\zeta = e^{iq_x}$ and $\phi = e^{iq_y}$. This matrix is easily diagonalized and has eigenvalues μ_1 and μ_2 given by

$$\mu_1 = M_2 + 2M_1(2 + \cos q_x + \cos q_y) \tag{2.37a}$$

and

$$\mu_2 = M_2$$
 , (2.37b)

respectively. Note that while the degeneracy of the larger eigenvalue branch is broken in second order that of the lower branch remains unbroken.

More generally, for a (d-1)-dimensional layer, the largest branch of eigenvalues in the spectrum of $M^{(+)}(\mathbf{q})$ is given by

$$\mu_1(\vec{q}) = M_2 + 2M_1 \left(1 + \sum_{l=1}^{d-1} \cos(q_l) \right) \quad . \tag{2.38}$$

This suffices to enable one to write the uppermost branch of eigenvalues in the bound-pair spectrum of K to second order in u_{\parallel} as

$$\lambda_{2a}[\vec{q}; 1(+)] = \Lambda_{2a}(+) + \mu_1(\vec{q}) + O(u_{\parallel}^4) \quad . \qquad (2.39)$$

This completes the treatment of the finite-field low-temperature spectrum. The most significant feature obtained is that both the first and second bands of eigenvalues below λ_0 have a single-particle character.

D. Zero-Field Low-Temperature Spectrum in Three or More Dimensions

In zero field, because of the up-down symmetry of the Ising Hamiltonian, the states $|\Phi(\pm)\rangle$ are the degenerate eigenstates of K₂ with largest eigenvalue. Indeed, as is seen from (2.17) all the states $|\tilde{r}_1, \ldots, \tilde{r}_n(+)\rangle$ and $|\tilde{r}_1, \ldots, \tilde{r}_n(-)\rangle$ become pairwise degenerate in zero field, and the spectrum of <u>K</u>₂ doubles up. In addition in zero field the size of eigenvalues is no longer a strictly decreasing function of particle number. In particular, with nearest-neighbor interactions on the three-dimensional simple cubic lattice the eigenstates $|\tilde{r}, \tilde{r} + \delta, \tilde{r} - \delta(\pm)\rangle$ and the states of four particles on a nearest-neighbor square are degenerate with the states $|\tilde{r}_1, \tilde{r}_2(\pm)\rangle$ of two separated particles. The zero-field zero-, one-, and twoparticle eigenvalues are obtained from (2.16a)-(2.16d) by taking the limit *h* tending to zero. The three- and four-particle eigenvalues are given by

$$\Lambda_{3,a}(\pm) = t_{\parallel}^{N} \exp\{\frac{1}{2} \left[(N-12)\hat{\varphi}(0) + 8 \right] K_{\perp} \} , \quad (2.40a)$$

$$\Lambda_{3,b}(\pm) = t_{\parallel}^{N} \exp\{\frac{1}{2} \left[(N-12)\hat{\varphi}(\vec{0}) + 4 \right] K_{\perp} \}, \quad (2.40b)$$

$$\Lambda_{3,c}(\pm) = t_{\parallel}^{N} \exp\{\frac{1}{2} \left[(N - 12)\hat{\varphi}(\vec{0}) \right] K_{\perp} \} , \qquad (2.40c)$$

$$\Lambda_{4,a}(\pm) = t_{\parallel}^{N} \exp\{\frac{1}{2} \left[(N - 16)\hat{\varphi}(\overline{0}) + 16 \right] K_{\perp} \} ,$$
(2.40d)

and so on. Table I illustrates the uppermost part of the zero-field spectrum of \underline{K}_2 . In three dimensions $\hat{\varphi}(\overline{0}) = 4$, and thus $\frac{1}{2}(N-\overline{12})\hat{\varphi}(\overline{0}) + 8$ is equal to $\frac{1}{2}(N-8)\hat{\varphi}(\overline{0})$, and to $\frac{1}{2}(N-16)\hat{\varphi}(\overline{0}) + 16$, so that $\Lambda_{2,b}(\pm)$, $\Lambda_{3,a}(\pm)$, and $\Lambda_{4,a}(\pm)$ are degenerate. Note that at fixed particle number n_i the levels are dictionary ordered: $\Lambda_{n,a}(\pm) > \Lambda_{n,b}(\pm) > \Lambda_{n,c}(\pm)$, and so forth.

At low temperatures $|\vec{r}_1, \ldots, \vec{r}_n(+)\rangle$ and $|\vec{r}, \ldots, \vec{r}_n(-)\rangle$ do not mix until very high order in

$\Lambda_0(\pm)$	{ (±) }	2 states
$\Lambda_1(\pm)$	Ť (±) ⟩	2N states
$\Lambda_{2a}(\pm)$	$ \mathbf{\dot{r}},\mathbf{\ddot{r}}+\vec{\delta}(\pm)\rangle$	$N\hat{arphi}(\vec{0})$ states
$\Lambda_{2b}(\pm)$	$ \vec{\mathbf{r}}_1, \vec{\mathbf{r}}_2(\pm)\rangle$	$N[N-1-\hat{arphi}(ar{0})]$ states
$\Lambda_{3a}(\pm)$	$ \mathbf{\dot{r}},\mathbf{\ddot{r}}+\mathbf{\ddot{\delta}},\mathbf{\ddot{r}}+\mathbf{\ddot{\gamma}}(\pm)\rangle$	$N[\hat{\varphi}(\overline{0})^2 - 2\hat{\varphi}(\overline{0})]$ states
$\Lambda_{3b}(\pm)$	$ \mathbf{\tilde{r}}_1,\mathbf{\tilde{r}}_1+\mathbf{\tilde{\delta}},\mathbf{\tilde{r}}_2(\pm)\rangle$	$N(N-2)\hat{\varphi}(\vec{0})$ states
$\Lambda_{3c}(\pm)$	$ \bar{r}_{1}, \bar{r}_{2}, \bar{r}_{3}(\pm)\rangle$	$\frac{1}{3}N(N-1)(N-2) - N\hat{\varphi}(\vec{0})[N-4+\hat{\varphi}(\vec{0})] \text{ states}$
$\Lambda_{4a}(\pm)$	$ \mathbf{\tilde{r}}_{1},\mathbf{\tilde{r}}_{1}+\mathbf{\tilde{\delta}},\mathbf{\tilde{r}}_{1}+\mathbf{\tilde{\gamma}},\mathbf{\tilde{r}}_{1}+\mathbf{\tilde{\delta}}+\mathbf{\tilde{\gamma}}\rangle$	2N states
•		
•		
•		
$\Lambda_{nl}(\pm)$		

TABLE I. Zero-field spectrum of \underline{K}_2 : (i) in three dimensions, $\Lambda_{2b}(\pm) = \Lambda_{3a}(\pm) = \Lambda_{4a}(\pm) > \Lambda_{3b}(\pm)$; (ii) in four dimensions, $\Lambda_{3b}(\pm) = \Lambda_{4a}(\pm) > \Lambda_{3c}(\pm)$.

 u_{\parallel} because each order of u_{\parallel} is capable of changing the particle number by 1, and the above states differ in particle number by O(N-2n). Therefore, the spectrum of K will be composed of two largely noninteracting spectra. Of course when *n* becomes comparable to $\frac{1}{2}N$ the two spectra mix strongly even at low temperatures. However, since such states affect neither the thermodynamics, nor the decay of correlation, they are essentially uninteresting.^{1,2}

The zero-field eigenvalue spectrum may be obtained as the h=0 limit of the finite-field results obtained in Sec. IIC. Furthermore, the eigenstates $|\lambda_0(-)\rangle$, $|\lambda_1(\vec{q})(-)\rangle$, and so on are obtained from the corresponding type (+) eigenstates simply by replacing the (+) label by (-) on all zerothorder states involved.

It is easily seen that one cannot use this prescription to obtain the zero-field spectrum in two dimensions. In this case the layers are linear chains with coordination $\hat{\varphi}(\bar{0}) = 2$. (This is true not only on the square net, but also generally—for example on the triangular and honeycomb nets as well.) Now, in the perturbation expansion with $h \neq 0$, the single particle was found above to mix in second order with states of two nearest-neighbor particles. The mixing coefficient involves an "energy denominator"

 $(\exp\{[2\hat{\varphi}(\mathbf{0})-4]K_{\perp}+2h\}-1)^{-1}$.

When $\hat{\varphi}(\overline{0})$ is equal to 2 and *h* is zero, this coefficient diverges signaling the breakdown of the perturbation scheme. This breakdown occurs because, with h=0, and $\hat{\varphi}(\overline{0})=2$, the zeroth-order single-particle states are degenerate with states of two neighboring particles. Indeed they are degenerate with states of *n* particles clustered in a chain (the number of wrong bonds being two for all such states). Whence the necessity of treating the h=0, d=2 case separately.

In Paper I, ¹ it was noted that for a system with strictly finite layers, a pair-correlation function $G_{AB}(\vec{\mathbf{R}})$ decayed according to

$$G_{AB}(\mathbf{\bar{R}}) \approx \langle \lambda_0 | \underline{A}(\mathbf{\bar{0}}) | \lambda_1 \rangle \langle \lambda_1 | \underline{B}(\mathbf{\bar{r}}_1) | \lambda_0 \rangle \langle \lambda_1 / \lambda_0 \rangle^{|\mathbf{r}_{\parallel}|} ,$$
(2.41)

where $\vec{R} = r_{\parallel}\hat{z} + \vec{r}_{\perp}$. However, when the layer size tends to infinity the eigenvalue λ_1 becomes generally the leading edge of a band of such eigenvalues, and one must integrate over this band of levels to obtain the decay of correlation¹:

$$G_{AB}(\vec{\mathbf{R}}) \approx \int_{\Omega} d\xi \langle \lambda_0 | \underline{A}(\vec{0}) | \lambda_1(\xi) \rangle \\ \times \langle \lambda_1(\xi) | \underline{B}(\vec{\mathbf{r}}_1) | \lambda_0 \rangle e^{-|\mathbf{r}_1| \cdot \hat{\mathbf{k}}(\xi)} \quad . \qquad (2.42)$$

In (2.42) ξ is the band index, and the inverse correlation length $\hat{\kappa}(\xi)$ is defined, as in Paper II,² by

$$\hat{\kappa}(\xi) = \ln[\lambda_0 / |\lambda_1(\xi)|] \quad . \tag{2.43}$$

At high temperatures² the index ξ was given by the (d-1)-dimensional vector \mathbf{q} which ranges over the first Brillouin zone of the lattice reciprocal to the layer lattice—as seen above in the treatment of $\lambda_1[(\mathbf{q})(+)]$, this is also the case at low temperatures (except for d=2 and h=0).

Using Eq. (2.43) and the results of Sec. II C, the fundamental inverse length $\hat{\kappa}^*(\bar{\mathbf{q}})$ may be written

$$\hat{t}^{*}(\vec{q}) = 2[K_{1}\hat{\varphi}(\vec{0}) + h] + u_{\parallel}^{2} \left[1 + \frac{2\Lambda_{2b}(+)}{\Lambda_{1}(+) - \Lambda_{2b}(+)} - 2\left(\frac{\Lambda_{2a}(+)}{\Lambda_{1}(+) - \Lambda_{2a}(+)} - \frac{\Lambda_{2b}(+)}{\Lambda_{1}(+) - \Lambda_{2b}(+)}\right)\right]$$

$$\times \left(\hat{\varphi}(\vec{0}) + \sum_{l=1}^{d-1} \cos(q_l) \right) + O(u_{ll}^4) \quad . \quad (2.44)$$

In zero field, $\hat{\kappa}^{+}(\mathbf{\bar{q}}) = \hat{\kappa}^{-}(\mathbf{\bar{q}}) = \hat{\kappa}(\mathbf{\bar{q}})$, and $\hat{\kappa}(\mathbf{\bar{q}})$ is given by (2.44) with h = 0. Of course, the inverse correlation length κ is given by

$$\kappa = \lim_{\mathbf{\hat{q}} \to 0} \hat{\kappa}^*(\mathbf{\hat{q}}). \tag{2.45}$$

As shown in Paper I, 1 this is the *universal* inverse length for the decay of pairwise correlation functions defined on the system.

E. Zero-Field Low-Temperature Spectrum in Two Dimensions

The very interesting case of the zero-field twodimensional Ising transfer matrix will be analyzed in this section. The perturbation treatment will be similar to that employed in the finite-field case, with, however, the exception that the first band below the zero-particle level will have a two-particle rather than single-particle character. Indeed the most convenient picture for treating this problem is one in which the particles are wrong $[\uparrow - \downarrow \text{ or } \downarrow - \uparrow]$ bonds in the layer. Then it turns out that with periodic boundary conditions, there can only be states with an even number of wrong bonds. (With free-edge boundary conditions there *can* be an odd number of particles associated with surface states. Thus, for example, the single-particle band reappears. However, it is easily seen that this band does *not* affect the decay of bulk correlation functions. In any case, such surface effects will be dealt with in a forthcoming work and will not be considered further herein.)

Let us reexamine the form of \underline{K}_2 , the intralayer matrix:

$$\underline{\mathbf{K}}_{2} = t_{\parallel}^{N} \exp\left(K_{\perp} \sum_{r=1}^{N} \underline{\sigma}^{\mathbf{z}}(r) \underline{\sigma}^{\mathbf{z}}(r+1)\right) \quad . \tag{2.46}$$

The sum over spin operators $\underline{\sigma}^{\mathbf{z}}(r)\underline{\sigma}^{\mathbf{z}}(r+1)$ may be regarded as a function constructed by examining every pair of neighboring spins, and assigning to the pair the value +1 if they are co-aligned $[\bigstar - \bigstar$ or $\bigstar - \bigstar]$, or the value -1 if they are antialigned $[\bigstar - \bigstar$ or $\bigstar - \bigstar]$, and by then summing this assigned number over all pairs in the layer. If *n* is the number of wrong bonds (antialigned pairs), and *N* the number of sites in a layer, then

$$\sum_{r=1}^{N} \underline{\sigma}^{\mathbf{z}}(r) \underline{\sigma}^{\mathbf{z}}(r+1) = N - 2n \quad . \tag{2.47}$$

Any state with a definite number n of such wrong bonds is an eigenstate of \underline{K}_2 with eigenvalue Λ_n given by

$$\Lambda_n = t_{\perp}^N e^{(N-2n)K_{\perp}} \quad . \tag{2.48}$$

As before there are two zero-particle states; namely, $|\Phi(+)\rangle = |\uparrow\uparrow\cdots\downarrow\downarrow\rangle$ and $|\Phi(-)\rangle$

 $= | \downarrow \downarrow \cdots \downarrow \downarrow \rangle$. These two are the degenerate eigenstates of K_2 of largest eigenvalue.

With periodic boundary conditions there can be no single-particle states. For example, because the first and Nth sites are nearest neighbors of one another, even the state $|\uparrow\uparrow-\downarrow\cdots\downarrow\downarrow\rangle$ actually contains two particles or wrong bonds; the notationally obvious one together with the implied wrong bond between the first and last spins. It will be convenient to label the bonds sequentially using the convention that the *r*th bond connects the *r*th and (r+1)th layer sites. Note that there are two distinct particle types: $(\uparrow-\downarrow)$ labeled as (+)particles, and $(\downarrow-\downarrow)$ labeled as (-) particles.

With these conventions it is easily seen that there are $2\binom{N}{n}$ *n*-particle states, where $\binom{N}{n}$ is the binomial coefficient. The $\binom{N}{n}$ arises because there are $\binom{N}{n}$ ways of placing *n* identical particles in *n* of *N* identical boxes. The two arises because there are two distinct types of particles. [It is crucial to this argument that (+) and (-) particles necessarily interlace each other.] For an *N*-site layer there are 2^N spin configurations of the layer. To show that the above particle enumeration generates all 2^N configurations, it suffices to show that

$$2\sum_{l=0}^{N/2} \binom{N}{2l} = 2^{N} \quad . \tag{2.49}$$

To do so, consider the binomial expansion

$$(1+x)^{N} + (1-x)^{N} = 2 \sum_{l=0}^{N/2} {N \choose 2l} x^{l}$$
 (2.50)

With x equal to 1, (2.50) produces the desired result (2.49).

The effect of the perturbation $[(\underline{K}_1 - \underline{I})\underline{K}_2]$ on the states and levels of \underline{K}_2 may now be determined. As noted above, with periodic boundary conditions only states with even particle numbers need be considered. Since the type-(+) and type-(-) particles alternate, if the first particle encountered in the layer is type (+), the last particle encountered is necessarily type (-), and vice versa. Thus, to uniquely specify the eigenstates of \underline{K}_2 it suffices to note all the particle encountered with the type of the first particle encountered when moving across the layer from left to right. For example, the state $|r_1, r_2: (-)\rangle$ is of the form $| \bigstar \cdots \bigstar - \bigstar \cdots \bigstar - \bigstar \rangle$.

The first-order term in the perturbation may be written

$$[(\underline{\mathbf{K}}_{1}-\underline{\mathbf{I}})\underline{\mathbf{K}}_{2}]_{1} = t_{\parallel}^{N} \exp\left(NK_{\perp}-2K_{\perp}\sum_{l=1}^{N} [\underline{\mathbf{n}}^{*}(l)+\underline{\mathbf{n}}^{-}(l)]\right)$$
$$\times u_{\parallel}\sum_{l=1}^{N} \underline{\sigma}^{x}(l) \quad , \quad (2.51)$$

where $\underline{n}^{*}(l)$ is the number operator for type-(±) particles and $\underline{\sigma}^{*}(l) = \underline{\sigma}^{*}(l) + \underline{\sigma}^{-}(l)$, as above. One easily sees that

$$\sum_{l=1}^{N} \underline{n}^{+}(l) = \sum_{l=1}^{N} \underline{n}^{-}(l) = \frac{1}{2} \sum_{l=1}^{N} [\underline{n}^{+}(l) + \underline{n}^{-}(l)] . \quad (2.52)$$

The only off-diagonal terms in (2.51) are those involving $\underline{\sigma}^{x}(l)$; so it is useful to note the effect of this operator on the state of K_2 . First consider its effect upon the vacuum states:

$$\underline{\sigma}^{x}(l) \left| \Phi(\pm) \right\rangle = \delta(l, 1) \left| 1, N: (\mp) \right\rangle$$

+
$$[1 - \delta(l, 1)] | l - 1, l : (\pm) \rangle$$
, (2.53)

which means that the first-order diagrams only link the vacuum with nearest-neighbor states of two particles. Next consider $\underline{\sigma}^{x}(l)$ acting on states with two neighboring particles:

$$\underline{\sigma}^{x}(l) | r, r+1: (\pm) \rangle = \delta(r, l) | r-1, r+1: (\pm) \rangle + \delta(r+1, l) | \Phi(\pm) \rangle + \delta(l, r+2) | r, r+2: (\pm) \rangle + [1 - \delta(r, l) - \delta(l, r+1) - \delta(l, r+2)] | l-1, l, r, r+1: (\pm) \rangle .$$
(2.54)

The nearest-neighbor two-particle states are connected to the vacuum states, second-neighbor two-particle states, and to the four-particle states consisting of two disconnected nearest-neighbor pairs, by the per-turbation. For second-neighbor two-particle states,

$$\frac{g^{x}(l)|r-1,r+1:(\pm)\rangle = \delta(l,r-1)|r-2,r+1:(\pm)\rangle + \delta(r,l)|r,r+1:(\pm)\rangle + \delta(l,r+2)|r-1,r+2;(\pm)\rangle }{+\delta(l,r+1)|r-1,r:(\pm)\rangle + [1-\delta(r-1,l)-\delta(r,l)\delta(l,r-1)-\delta(l,r+2)]} \times |l-1,l,r-1,r+1:(\pm)\rangle .$$
(2.55)

For third or further neighbors, one has

$$\underline{\sigma}^{x}(l) | r, r': (\pm) \rangle = \delta(l, r) | r - 1, r': (\pm) \rangle + \delta(l, r + 1) | r + 1, r': (\pm) \rangle + \delta(l, r' + 1) | r, r' + 1: (\pm) \rangle \\ + \delta(l, r') | r, r' - 1: (\pm) \rangle + [1 - \delta(l, r) - \delta(l, r + 1) - \delta(l, r') - \delta(l, r' + 1)] | l - 1, l, r, r': (\pm) \rangle .$$

$$(2.56)$$

In (2.53)-(2.56), when *l* is equal to 1, $\underline{\sigma}^{x}(l)$ changes type-(+) states into type-(-) states, and vice versa. For example, the state $| \uparrow \uparrow \cdots \uparrow - \downarrow - \uparrow \cdots \uparrow \rangle$, a type-(+) state is transformed by $\underline{\sigma}^{x}(1)$ into $| \downarrow - \uparrow \cdots \uparrow - \downarrow - \uparrow \cdots \uparrow \rangle$, a type-(-) state. Thus, since $\underline{\sigma}^{x}(l)$ mixes the (+) and (-) states even in first order, the first-order diagrams which arise in breaking the degeneracy of the (2n)-particle levels are *not* block diagonal in $\binom{N}{2n}$ -dimensional blocks. But, if one chooses proper linear combinations of (+) and (-) states, the first-order matrices will break into two equally dimensioned blocks. Consider

$$|r_{1}, r_{2}, \cdots r_{2n}; S\rangle = \frac{1}{\sqrt{2}} [|r_{1}, \cdots, r_{2n}; (+)\rangle + |r_{1}, \cdots, r_{2n}; (-)\rangle] , \quad (2.57)$$
$$|r_{1}, r_{2}, \cdots, r_{2n}; A\rangle = \frac{1}{\sqrt{2}} [|r_{1}, \cdots, r_{2n}; (+)\rangle - |r_{1}, \cdots, r_{2n}; (-)\rangle] , \quad (2.58)$$

which are symmetrical and antisymmetrical 2n-particle states, respectively. It is clear that every symmetrical state is orthogonal to every antisymmetrical state. Further it is seen that $[(\underline{K}_1 - \underline{I})\underline{K}_2]$ does *not* mix these two kinds of states. The imposition of cyclic boundary conditions within

the layer is equivalent to taking the first and (N+1)th bonds to be the same bond. However, with the above labeling convention one has

$$|x, N+1: (\pm)\rangle = |1, x: (\mp)\rangle$$
 . (2.59)

This does not affect the boundary conditions of the symmetrical states. But for the antisymmetrical states (2.59) implies that

$$|x, N+1:A\rangle = -|1, x:A\rangle$$
 . (2.60)

That is, the antisymmetrical states satisfy antiperiodic boundary conditions! Two *noninteracting* sets of states of (2n) *identical* particles have thus been obtained, the one satisfying periodic and the other satisfying antiperiodic boundary conditions.

Before finding the low-order eigenstates and eigenvalues, it will prove useful to show that $u_{\parallel}\sum_{l=1}^{N} \underline{\sigma}^{x}(l)$ may be written as a two-body operator in this picture. It is already seen from (2.53)-(2.56) that such an isomorphism must be possible since the effect of this operator upon the states of \underline{K}_{2} is always to create or destroy two particles, or to leave the particle number unchanged. [With free edges no such isomorphism can be obtained since $\underline{\sigma}^{x}(l)$ is then capable of creating or destroying a single particle on either the first or Nth bonds.]

Let us introduce creation and annihilation operators for symmetrical and antisymmetrical par-

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ticles. Denote by $\underline{\psi}_{S}(r)$ and $\underline{\psi}_{S}^{\dagger}(r)$ the destruction and creation operators for a symmetric particle at site r; similarly denote by $\underline{\psi}_{A}(r)$ and $\underline{\psi}_{A}^{\dagger}(r)$ the like operators for an antisymmetric particle. Letting P(=A, S) be the parity, the eigenstates of K_{2} may be written

$$|r_1, r_2, \ldots, r_{2n}; P\rangle = \underline{\psi}_P^{\dagger}(r_1) \cdots \underline{\psi}_P^{\dagger}(r_{2n}) |\Phi: P\rangle \quad .$$
(2.61)

These states are even under exchange of particles and there can be no more than one particle per bond. Having noted these facts, one sees the algebra of $\{\underline{\psi}_P(r)\}$ to be the same Pauli algebra as obeyed by $\underline{\sigma}^{*}(r)$ [(2.10)-(2.13)] and by the operators $\{\underline{\psi}(\mathbf{\tilde{r}})\}$ employed in the high-temperature analysis of Paper II.² The operator $\underline{\psi}_P(r)$ projects onto the subspace of parity P and then destroys a particle at site r.

In terms of these operators for symmetric and antisymmetric states, the perturbation takes the form

$$u_{\parallel} \sum_{l=1}^{N} \underline{\sigma}^{x}(l) = u_{\parallel} \sum_{P} \sum_{l=1}^{N} [\underline{\psi}_{P}(l) + \underline{\psi}_{P}^{\dagger}(l)] \times [\psi_{P}(l+1) + \underline{\psi}_{P}^{\dagger}(l+1)] . \quad (2.62)$$

In verifying the correctness of (2.62), difficulty only arises in handling the boundary conditions of the antisymmetric states. However, close scrutiny shows that (2.60) and (2.62) enable one to exactly reproduce the effect of $(K_1 - I)K_2$. For, consider the effect of $\sigma^{x}(l)$ on a general (2n)-particle state. If neither \overline{l} nor l-1 is occupied, it creates a particle on each of these bonds. If only one of these sites is unoccupied, it destroys the existing particle and creates a particle on the previously unoccupied site (thereby simply shifting the original particle one site, and leaving the particle number unchanged). When both l-1 and *l* are occupied, $\sigma^{x}(l)$ destroys both particles. This is exactly the effect of $[\psi_P(l) + \psi_P^{\dagger}(l)] \cdot [\psi_P(l-1)]$ $+\psi_P^{\dagger}(l-1)$]. Examination of the boundary condition (2.60)—which says that $|1, r_1, \dots, r_l: A\rangle$ is equal to $-|r_1, \ldots, r_l, N+1:A\rangle$ — completes the verification of (2.62).

It is useful to introduce the number operator,

$$n_P(l) = \psi_P^{\dagger}(l)\psi_P(l)$$
 . (2.63)

Using the above definitions, one can verify that

$$\sum_{P} \sum_{l=1}^{N} \underline{n}_{P}(l) = \sum_{l=1}^{N} [\underline{n}^{*}(l) + \underline{n}^{-}(l)] , \qquad (2.64)$$

so that if <u>P</u> is the projector onto the subspace of parity <u>P</u> [recall that $\underline{\psi}_P(l)$ and $\underline{\psi}_P^{\dagger}(l)$ are defined so as to project onto this subspace] the transfer matrix can be written

$$\underline{\mathbf{K}} = t_{\parallel}^{N} \exp \left[K_{\perp} \sum_{P} \left(N\underline{\mathbf{P}} - 2 \sum_{l=1}^{N} \underline{\mathbf{n}}_{P}(l) \right) \right]$$

$$\times \exp\left(u_{\parallel} \sum_{P} \sum_{l=1}^{N} \left[\underline{\psi}_{P}(l) + \underline{\psi}_{P}^{\dagger}(l)\right] \\ \times \left[\underline{\psi}_{P}(l+1) + \underline{\psi}_{P}^{\dagger}(l+1)\right]\right).$$

Therefore, K may be written

 $\underline{\mathbf{K}} = t_{\parallel}^{N} \underline{\mathcal{K}}_{A} \underline{\mathcal{K}}_{S} = t_{\parallel}^{N} \underline{\mathcal{K}}_{S} \underline{\mathcal{K}}_{A} ,$ with

$$\underline{\mathcal{K}}_{P} = \exp\left[K_{\perp}\left(N\underline{\mathbf{P}} - 2\sum_{l=1}^{N}\underline{\mathbf{n}}_{P}(l)\right)\right]$$

$$\times \exp\left(u_{\parallel}\sum_{l=1}^{N}\left[\underline{\psi}_{P}(l) + \underline{\psi}_{P}^{\dagger}(l)\right]$$

$$\times \left[\underline{\psi}_{P}(l+1) + \underline{\psi}_{P}^{\dagger}(l+1)\right]\right). \quad (2.67)$$

Note from (2.67) that \underline{x}_{4} operating on a symmetric state is equivalent to the identity operator I, as is \underline{x}_{s} operating on an antisymmetric state.

The form of the high-temperature zero-field transfer matrix was elucidated in Paper II^2 and is given by Eq. (2.31) of that paper with h=0, namely,

$$\underline{\mathbf{K}} = \mu_{*}^{N} \exp\left(-w_{\parallel} \sum_{l=1}^{N} \underline{\mathbf{n}}(l)\right) \exp\left(K_{1} \sum_{l=1}^{N} [\underline{\psi}(l) + \underline{\psi}^{\dagger}(l)] \times [\underline{\psi}(l+1) + \underline{\psi}^{\dagger}(l+1)]\right), \quad (2.68)$$

where $\underline{n}(l)[=\underline{\psi}^{\dagger}(l)\underline{\psi}(l)]$, $\underline{\psi}(l)$, and $\underline{\psi}^{\dagger}(l)$ are Pauli field operators with exactly the same algebra as $\underline{n}_{P}(l)$, $\underline{\psi}_{P}(l)$, and $\underline{\psi}_{P}^{\dagger}(l)$. Thus, for the square net, to within a temperature-dependent, but analytic, scale factor the low-temperature transfer matrix—given by (2.66) with (2.67)—has *exactly* the same functional form as the high-temperature matrix—given by (2.68). [This is, of course, true as long as one operates on states of definite (A or S) parity.] Let us introduce the fundamental variable K_{\pm}^{*} by

$$\ln[\coth(K_{\parallel}^{*})] = 2K_{\perp} \quad . \tag{2.69}$$

Further let K_1^* be defined by

$$u_{\parallel} = K_{\perp}^{*}$$
, (2.70)

so that

$$2K_{\mu} = \ln[\coth(K_{+}^{*})] \quad . \tag{2.71}$$

Recall now that in zero field, $w_{\parallel} = \ln[\coth(K_{\parallel})]$. The low-temperature matrix $\underline{\mathcal{K}}_{P}$ thus takes the form

$$\begin{split} \underline{\mathfrak{K}}_{P} &= e^{NK_{1}\underline{\mathbf{P}}} \exp\left(-\ln[\coth(K_{\parallel}^{*})]\sum_{l=1}^{N}\underline{\mathbf{n}}_{P}(l)\right) \\ &\times \exp\left(K_{1}^{*}\sum_{l=1}^{N}\left[\underline{\psi}_{P}(l) + \underline{\psi}_{P}^{\dagger}(l)\right] \\ &\times \left[\underline{\psi}_{P}(l+1) + \underline{\psi}_{P}^{\dagger}(l+1)\right]\right), \quad (2.72) \end{split}$$

(2.65)

(2.66)

so that operating on states of given parity, the total transfer matrix K becomes

$$(\underline{\mathbf{K}})_{P} = (t_{\parallel}e^{K_{\perp}})^{N} \exp\left(-\ln\left[\coth(K_{\parallel}^{*})\right]\sum_{l=1}^{N}\underline{\mathbf{n}}(l)\right)$$
$$\times \exp\left(K_{\perp}^{*}\sum_{l=1}^{N} [\underline{\psi}(l) + \underline{\psi}^{\dagger}(l)][\underline{\psi}(l+1) + \underline{\psi}^{\dagger}(l+1)]\right),$$
(2.73)

which (given the substitution of μ_{+} for $t_{\parallel}e^{K_{\perp}}$) is exactly the high-temperature form for K. Note that this isomorphism allows one to calculate the critical temperature of the square Ising net.⁷ For, suppose that there is a unique critical point. Then it must be given by $K_{\perp}^{*} = K_{\perp}$ and $K_{\parallel}^{*} = K_{\parallel}$. Otherwise, by the duality transformation if there is a critical point for $K_{\perp} < K_{\perp}^{*}$ there must also be one of $K_{\perp}^{*} < K_{\perp}$, hence vitiating the assumption of a single critical point. Thus the critical point is located via

$$2K_{ic} = \ln[\coth(K_{ic})], \quad 2K_{ic} = \ln[\coth(K_{ic})] , \quad (2.74)$$

or, defining
$$V_{\parallel} = \tanh(K_{\parallel})$$
 and $V_{\perp} = \tanh(K_{\perp})$,

$$e^{-2K} = V_{\parallel c}, \quad e^{-2K} = V_{\perp c}$$
 (2.75)

For $K_{\parallel} = K_{\perp}$, this becomes $V_c = \sqrt{2} - 1$.⁷

This isomorphism enables one to calculate the low-temperature spectrum using the results of Paper II² for the high-temperature spectrum of K. At low temperatures the eigenvectors must be obtained to first order in u_{II} . However, all the other results may be taken directly over from Paper II.² Since the calculations involve straightforward perturbation theory only the results are presented.

The eigenstates $|\lambda_0; P\rangle$ for the largest two levels are given by

$$\lambda_{0}: P \rangle = |\Phi: P\rangle + u_{\parallel} (1 - e^{-4K_{\perp}})^{-1} \\ \times \sum_{r=1}^{N} |r, r+1: P\rangle + O(u_{\parallel}^{3}) , \quad (2.76)$$

and the eigenvalues are

$$\lambda_0(P) = t_{\parallel}^N e^{NK_\perp} \{ 1 + N u_{\parallel}^2 [e^{4K_\perp} - 1]^{-1} + O(u_{\parallel}^4) \} ,$$
(2.77)

and hence are degenerate in second order. The (2n)-particle eigenstates are constructed as follows: The zeroth-order states are $|\Psi(q_1, q_2, \ldots, q_{2n}): P\rangle$ with

$$\left|\Psi(q_{1},\ldots,q_{2n}):P\right\rangle = \sum_{r_{1}=1}^{N} \cdots \sum_{r_{2n}=1}^{N} \Psi_{q_{1}}\cdots q_{2n}(r_{1},\ldots,r_{2n})\right|r_{1},\ldots,r_{2n}:P\rangle \quad .$$
(2.78)

The wave function $\Psi_{q_1\cdots q_{2n}}(r_1,\ldots,r_{2n})$ is a symmetrized Slater determinant of running-wave states. Let $\varphi_q(r)$ be a running-wave state,

$$\varphi_q(r) = N^{-1/2} e^{iqr}$$
 (2.79)

Then,

$$\Psi_{a_{1}}\cdots_{a_{2n}}(r_{1},\ldots,r_{2n}) = \epsilon(q_{1},\ldots,q_{2n})$$
$$\times \epsilon(r_{1},\ldots,r_{2n}) \operatorname{Det} |\varphi_{a_{j}}(r_{j})|_{2n \times 2n} , \quad (2.80)$$

where $\text{Det}|A_{ij}|_{i \times i}$ is the determinant of the *l*-dimensional matrix <u>A</u> with coefficients A_{ij} and $\epsilon(x_1, \ldots, x_n)$ is the signature of the permutation of $(1, 2, \ldots, n)$ required to order x_1, \ldots, x_n in increasing size. Thus suppose the ordering is $x_{1'} < x_{2'} < \cdots < x_{n'}$ the signature $\epsilon(x_1, \ldots, x_n)$ will be positive (negative) if $(1', \ldots, n')$ is an even (odd) permutation of $(1, \ldots, n)$.

The wave function depends implicitly upon the parity through the boundary conditions. Recall that the symmetric (antisymmetric) states satisfy periodic (antiperiodic) boundary conditions. From Paper II, ^{2,8} recall that for $\Psi_{a_1} \cdots a_{2n} (r_1, \ldots, r_{2n})$ to satisfy periodic (antiperiodic) boundary conditions $\varphi_q(r)$ must satisfy antiperiodic (periodic) boundary conditions. Thus, for the symmetric states, q_i is restricted to

$$q_i = \pi (2n_i + 1)/N$$
, $n_i = 1, 2, ..., N$; $(P = S)$,
(2.81)

and for the antisymmetric states q_i verifies

$$q_i = 2\pi n_i / N$$
, $n_i = 1, 2, ..., N$; $(P = A)$. (2.82)

With these preliminaries the (2n)-particle eigenvalues are found to be

$$\lambda_{2n}(q_1, \dots, q_{2n}; P) = t_{||}^N e^{(N-4)K_{\perp}} \times \left(1 + 2u_{||} \sum_{l=1}^{2n} \cos(q_l) + O(u_{||}^3) \right) \qquad (2.83)$$

The two-particle eigenstates are given to first order as

$$\begin{aligned} |\lambda_{2}(q_{1}, q_{2}): P\rangle &= \left|\Psi(q_{1}, q_{2}): P\rangle + u_{\parallel}(1 - e^{-4K_{\perp}})^{-1} \\ &\times \sum_{r_{1}=1}^{N} \sum_{r_{2}=1}^{N} \sum_{r_{3}=1}^{N} \Psi_{q_{1}q_{2}}(r_{1}, r_{2}) \left|r_{1}, r_{2}, r_{3}, r_{3}+1: P\rangle \\ &- 2u_{\parallel}(e^{4K_{\perp}}-1)^{-1} \sum_{r=1}^{N} \Psi_{q_{1}q_{2}}(r, r+1) \left|\Phi: P\rangle + O(u_{\parallel}^{2}) \end{aligned} \end{aligned}$$

Note that the eigenvalues $\lambda_{2n}(q_1, \ldots, q_{2n}; A)$ and $\lambda_{2n}(q_1, \ldots, q_{2n}; S)$ differ slightly since the wave vectors q_i differ by $O(\pi/N)$ for the two symmetries.

As N tends to infinity this difference disappears and the levels become fully degenerate with one another. The qualitative features of the zeroand two-particle spectra are presented in Fig. 2.

The fundamental inverse correlation length $\hat{\kappa}(q_1, q_2; P)^{1,2,3}$ is

$$\hat{\kappa}(q_1, q_2; P) \equiv \ln[\lambda_0(P) / |\lambda_2(q_1, q_2; P)|]$$

= $4K_1 - 2u_{\parallel}[\cos(q_1) + \cos(q_2)] + O(u_{\parallel}^3)$,
(2.85)

where q_1 and q_2 verify (2.81) and (2.82) in the symmetric and antisymmetric cases, respectively.

This completes the treatment of the low-temperature zero-field two-dimensional transfermatrix spectrum. With free-edge boundary conditions the results are changed by the appearance of states with odd particle number associated with surface states. However, as will be shown in Paper IV of this series such states do not affect the results derived herein for the decay of correlation within the bulk. Finally, note that even with cyclic boundary conditions the addition of secondand/or further-neighbor interactions fundamentally alters these results. For example with secondneighbor forces the states of a single overturned spin (called herein nearest-neighbor two-particle states) form a single-particlelike band which lies above the states with two nearest-neighbor overturned spins. Below this is the remainder of the two-particle states (states with three or more overturned spins in a row). The important point is that the first three levels are *exactly* like those with d equal to or greater than 3. Thus, the analysis of the spectrum and the low-temperature decay of correlations follow in detail that presented for h = 0, d equal to or greater than 3. In particular, the decay of correlation is then found to be OZ.

In Sec. III the various correlation functions are obtained in terms of the states and levels calculated in this section.

III. ASYMPTOTIC DECAY OF CORRELATION AT LOW TEMPERATURES

A. Introduction

In this section the results of Sec. II are used to obtain the asymptotic decay of net-pair-correlation functions at low temperatures. The division of the calculations follows the same lines as the division of the derivation of the various spectra of K in Sec. II.

In Sec. III B the decay of correlation in a nonzero field is considered for arbitrary dimension d. As will be seen below, the decay of an arbitrary net-pair-correlation function then turns out to be OZ in form.

The zero-field decay in three or more dimensions is considered in IIIC. Again the decay of correlation will be found to be OZ. Finally, IIID comprises a treatment of the decay of correlation functions in two dimensions and zero field. The decay of these correlation functions is found to be given by the non-OZ form $R^{-2}e^{-\kappa R}$ found by Kadanoff⁴ and by Wu.⁴

B. Decay of Correlation in Finite Field

The net-pair-correlation function $G_s(\mathbf{\bar{R}}, h)$ is defined by

$$G_{s}(\vec{\mathbf{R}},h) = \langle \delta S^{\boldsymbol{z}}(\vec{\mathbf{0}},0) \delta S^{\boldsymbol{z}}(\vec{\mathbf{r}}_{\perp},\boldsymbol{r}_{\parallel}) \rangle \quad , \qquad (3.1)$$

where $\mathbf{\vec{R}} = \mathbf{\vec{r}}_{\perp} + r_{\parallel} \hat{z}$, exactly as in Paper II.² Again, the asymptotic decay of correlation is determined by the first band of eigenvectors below the largest level, together with the largest level itself. That is, as $|r_{\parallel}|$ tends to infinity:

$$G_{s}(\vec{\mathbf{R}},h) \approx \sum_{\vec{\mathbf{q}}} e^{-|\mathbf{r}_{\parallel}|\hat{\mathbf{k}}^{+}(\vec{\mathbf{q}})} \langle \lambda_{0}(+) | \underline{\sigma}^{\varepsilon}(\vec{\mathbf{0}}) | \lambda_{1}(\vec{\mathbf{q}})(+) \rangle \\ \times \langle \lambda_{1}(\vec{\mathbf{q}})(+) | \underline{\sigma}^{\varepsilon}(\vec{\mathbf{r}}_{\perp}) | \lambda_{0}(+) \rangle , \quad (3.2)$$

where $\hat{\kappa}^*(\vec{q})$ given by Eq. (2.44), $|\lambda_0(+)\rangle$ by Eq. (2.19), and $|\lambda_1(\vec{q})(+)\rangle$ by Eq. (2.27).

Recall that K_1 and K_2 do not commute, so that



 $[(\underline{\mathbf{K}}_1 - \underline{\mathbf{I}})\underline{\mathbf{K}}_2]_n$ is not Hermitian. Whence $\langle \lambda_t(+) | \cdots \rangle$ is not given by the complex conjugate $\langle \cdots | \lambda_t(+) \rangle^*$ of $\langle \cdots | \lambda_t(+) \rangle$. Additionally, the energy denominators are modified in the expansion for the bra vectors just as they were in Paper II. Thus, $\Lambda_n(+)/[\Lambda_n(+) - \Lambda_m(+)]$ in the expansion for the ket vectors $|\cdots\rangle$ becomes $\Lambda_m(+)/[\Lambda_n(+) - \Lambda_m(+)]$ in the expansion for bra vectors $\langle \cdots |$. Then the matrix elements in (3.2) are easily evaluated as

$$\langle \lambda_{0}(+) | \underline{\sigma}^{z}(\vec{0}) | \lambda_{1}(\vec{q})(+) \rangle \langle \lambda_{1}(\vec{q})(+) | \underline{\sigma}^{z}(\vec{r}_{\perp}) | \lambda_{0}(+) \rangle$$

$$= \frac{4}{N} u_{\parallel}^{2} e^{-i\vec{q}\cdot\vec{r}_{\perp}} \frac{\Lambda_{1}(+)\Lambda_{0}(+)}{\Lambda_{0}(+) - \Lambda_{1}(+)} + O(u_{\parallel}^{3}) .$$

$$(3.3)$$

Let us introduce the quantities $a(h, K_{\perp})$ and $b(h, K_{\perp})$ via

$$a(h, K_{1}) = \frac{\Lambda_{2a}(+)}{\Lambda_{1}(+) - \Lambda_{2a}(+)} - \frac{\Lambda_{2b}(+)}{\Lambda_{1}(+) - \Lambda_{2b}(+)}$$
(3.4)

and

$$b(h, K_{\perp}) = \frac{2\Lambda_{2b}(+)}{\Lambda_{1}(+) - \Lambda_{2b}(+)} , \qquad (3.5)$$

respectively. Then $\hat{\kappa}^*(\vec{q})$ may be expressed as

$$\widehat{\kappa}^{*}(\overrightarrow{\mathbf{q}}) = \left[2[h + K_{\perp}\widehat{\varphi}(\overrightarrow{\mathbf{0}})] + u_{\parallel}^{2} \left(1 + b(h, K_{\perp}) - 2a(h, K_{\perp}) - 2a(h, K_{\perp}) \right) - 2a(h, K_{\perp}) \sum_{l=1}^{d-1} \cos q_{l} + O(u_{\parallel}^{3}) \right] \quad . \quad (3.6)$$

For $|\vec{\mathbf{r}}_1| \ll |r_1|$ the correlation function $G_s(\vec{\mathbf{R}}, h)$ becomes (as N tends to infinity)

$$G_{s}(\vec{\mathbf{R}},h) \approx 4u_{\parallel}^{2} \frac{\Lambda_{1}(+)\Lambda_{0}(+)}{[\Lambda_{0}(+)-\Lambda_{1}(+)]^{2}} \exp(-|r_{\parallel}| \{2[h+\hat{\varphi}(\vec{\mathbf{0}})K_{\perp}] + u_{\parallel}^{2}[1-b(h,K_{\perp})]\}) \int_{0}^{2\pi} \frac{d\theta_{1}}{2\pi} \cdots \int_{0}^{2\pi} \frac{d\theta_{d-1}}{2\pi} \times \sum_{l=1}^{d-1} \exp[2u_{\parallel}^{2} a(h,K_{\perp})|r_{\parallel}| \cos\theta_{l} - ir_{\perp l}\theta_{l}] . \quad (3.7)$$

As in Eq. (4.20) of Paper II,² the integrals

$$\int_{0}^{2\pi} \frac{d\theta}{2\pi} e^{i\nu\theta} e^{x\cos\theta}$$

are recognized as representations of the Bessel function $I_{\nu}(x)$.⁹ These integrals were asymptotically analyzed in that paper. [Equations (4.24) and (4.29) of Paper II present the relevant results for $x \rightarrow \infty$ and $\nu \rightarrow \infty$, respectively.] The results of that analysis are applied to Eq. (3.71) to yield

$$G_{s}(\vec{\mathbf{R}},h) \approx B_{d}(h) \frac{e^{-\kappa R}}{R^{(d-1)/2}} + \cdots \qquad (|r_{\parallel}| \to \infty) \quad ,$$
(3.8)

with

$$B_{d}(h) \approx \frac{4u_{\parallel}^{2} \Lambda_{1}(+) \Lambda_{0}(+)}{\left[\Lambda_{0}(+) - \Lambda_{1}(+)\right]^{2}} \left[4u_{\parallel}^{2} \pi a(h, K_{\perp})\right]^{-(d-1)/2} ,$$
(3.9)

and with κ given by the \bar{q} equal to zero limit of Eq. (3.6).

The second term in the asymptotic expansion of $G_s(\vec{\mathbf{R}}, h)$ vs $|\vec{\mathbf{R}}| \rightarrow \infty$ involves integration over the bound-pair bands. As noted above these bands have a "polarized" single-particle character so that they also lead to an OZ decay form $[\sim e^{-\kappa' R}/R^{(d-1)/2}]$ with, however, a decay length κ' given by

$$\kappa' = \kappa + 2[\hat{\varphi}(\vec{0}) - 1]K_{\perp} + 2h + O(u_{\parallel}^2) \quad . \tag{3.10}$$

At high temperatures and finite field, it was found that the four-spin functions, called energydensity pair-correlation functions, show OZ behavior.² A short calculation shows this also to be true at low temperatures. Let us introduce the energy-density correlation function

$$G_{\mathfrak{e}_{\perp}}(\vec{\mathbf{R}},h) = J_{\perp}^{2} \sum_{\vec{\mathbf{0}}} \langle \delta[S^{\mathbf{z}}(\vec{\mathbf{0}},\mathbf{0})S^{\mathbf{z}}(\vec{\mathbf{0}},\mathbf{0})] \\ \times \delta[S^{\mathbf{z}}(\vec{\mathbf{0}},r_{\parallel})S^{\mathbf{z}}(\vec{\mathbf{0}},r_{\parallel})] \rangle \quad . \quad (3.11)$$

Then as $|r_{\parallel}|$ tends to infinity,

$$G_{e_{\perp}}(\vec{\mathbf{R}},\hbar) \approx J_{\perp}^{2} \sum_{\vec{\delta}} \sum_{\vec{\delta}} e^{-\kappa + (\vec{\mathbf{d}}) |\mathbf{r}_{\parallel}|} \times \langle \lambda_{0}(+) | \underline{\sigma}^{x}(\vec{\mathbf{0}}) \underline{\sigma}^{x}(\vec{\delta}) | \lambda_{1}(\vec{\mathbf{q}})(+) \rangle \times \langle \lambda_{1}(\vec{\mathbf{q}})(+) | \underline{\sigma}^{x}(\vec{\mathbf{0}}) \underline{\sigma}^{x}(\vec{\delta}) | \lambda_{0}(+) \rangle .$$
(3.12)

The calculation of $G_{\epsilon_1}(\vec{\mathbf{R}}, h)$ rests upon the matrix elements which are found to be

$$\langle \lambda_{0}(+) | \underline{\sigma}^{\mathbf{z}}(\vec{\mathbf{0}}) \underline{\sigma}^{\mathbf{z}}(\vec{\mathbf{\delta}}) | \lambda_{1}(\vec{\mathbf{q}})(+) \rangle \langle \lambda_{1}(\vec{\mathbf{q}})(+) | \underline{\sigma}^{\mathbf{z}}(\vec{\mathbf{0}}) \underline{\sigma}^{\mathbf{z}}(\vec{\mathbf{\delta}}) | \lambda_{0}(+) \rangle$$

$$= \frac{8u_{i1}^{2} \Lambda_{0}(+) \Lambda_{1}(+)}{\Lambda_{0}(+) - \Lambda_{1}(+)} \sum_{\vec{\mathbf{\delta}}} \frac{1 + \cos \vec{\mathbf{q}} \cdot \vec{\mathbf{\delta}}}{N} + \cdots$$
(3.13)

With (3.12) and (3.13) as N tends to infinity the asymptotic analysis of Paper II, ² may be employed to show that

$$G_{e_1}(\vec{\mathbf{R}},h) \approx E_d(h) e^{-\kappa R} / R^{(d-1)/2}$$
, (3.14)

where, as above, κ is given by (3.6) with \bar{q} equal to zero, and $E_d(h)$ by

$$E_{d}(h) = 16J_{\perp}^{2}\hat{\varphi}(\vec{0})u_{\parallel}^{2} \frac{\Lambda_{0}(+)\Lambda_{1}(+)}{\Lambda_{0}(+) - \Lambda_{1}(+)} \times [4\pi u_{\parallel}^{2}a(h, K_{\perp})]^{-(d-1)/2} .$$
(3.15)

Thus, both $G_s(\vec{\mathbf{R}})$ and $G_{\epsilon_1}(\vec{\mathbf{R}})$ exhibit OZ behavior

at low temperatures in finite field. Indeed, OZ behavior is found generally in this case. Below it is shown that for $d \ge 3$, this remains true when h = 0.

C. Decay of Correlation in Zero Field in Three or More Dimensions

Let us now consider the decay of net-pair-correlation functions in three or more dimensions and zero magnetic field. The calculation will also be correct in two dimensions with second-neighbor interactions within the layer at sufficiently low temperatures. These correlation functions are chiefly distinguished from their high-temperature counterparts by the existence of nonzero matrix elements of the energy density between the largest eigenvector and the single-particle states. That is, at low temperatures and zero field the decay of energy-density and spin-net-pair-correlation functions are determined by the same band even in zero field.

At low temperatures the zero-field spectrum is made up of two degenerate noninteracting spectra. Further there are no nonzero matrix elements of $\underline{\sigma}_1^x \underline{\sigma}_2^x \cdots \underline{\sigma}_n^x$ connecting these two spectra for nmuch less than N. Therefore, one may write the excess-correlation function as

$$\begin{split} \langle \delta \underline{\mathbf{A}}(\mathbf{\vec{R}}_{0}) \delta \underline{\mathbf{B}}(\mathbf{\vec{R}}_{0} + \mathbf{\vec{R}}) \rangle &\approx \frac{1}{2} \sum_{\mathbf{\vec{q}}} e^{-|\mathbf{r}_{\parallel}|\mathbf{\hat{k}}(\mathbf{\vec{q}})} [\langle \lambda_{0}(+) | \underline{\mathbf{A}} | \lambda_{1}(\mathbf{\vec{q}})(+) \rangle \\ &\times \langle \lambda_{1}(\mathbf{\vec{q}})(+) | \underline{\mathbf{B}} | \lambda_{0}(+) \rangle \\ &+ \langle \lambda_{0}(-) | \underline{\mathbf{A}} | \lambda_{1}(\mathbf{\vec{q}})(-) \rangle \langle \lambda_{1}(\mathbf{\vec{q}})(-) | \mathbf{B} | \lambda_{0}(-) \rangle] , \end{split}$$

$$(3.16)$$

as $|r_{\parallel}|$ terms to infinity. $\hat{\kappa}(\mathbf{\bar{q}})$ is given by the zerofield limit of $\hat{\kappa}^{*}(\mathbf{q})$. Further the matrix elements have the same zero-field form for both the (+) and (-) spectra. Indeed, because of the symmetry of the spin operators, the zero-field limit [for (2n)-spin functions] is obtained by substituting h=0 into the results of the preceding section [that is, $\sigma^{\mathfrak{e}}(\mathbf{\vec{r}}) = 1 - 2n^{*}(\mathbf{\vec{r}}) = 2n^{-}(\mathbf{\vec{r}}) - 1$, where $n^{*}(\mathbf{\vec{r}})$ is the number (=0, 1) of type (\pm) particles at site \vec{r}]. Note that with definition (3.16), three-spin [or more generally (2n+1)-spin] expectations are zero since the contributions from the (+) and (-)spectra cancel. However, if one takes the limit as $h \rightarrow 0^+$ only the type-(+) spectrum enters, and the (2n+1)-spin functions are nonzero. This dependence on magnetic field boundary conditions is indicative of long-range order as discussed in Paper I.¹

We may thus write the spin and energy-density correlation functions as

$$G_s(\vec{\mathbf{R}}, h=0) \approx B_d(h=0) e^{-\kappa R} / R^{(d-1)/2}$$
 (3.17)

and

$$G_{e_{\perp}}(\vec{\mathbf{R}}, h=0) \approx E_d(h=0) e^{-\kappa R} / R^{(d-1)/2} ,$$
 (3.18)

respectively [the limit as $h \to 0$ and $\bar{q} \to 0$ of $\hat{\kappa}^*(\bar{q})$ yields κ]. It is emphasized that (3.17) and (3.18) also apply in two dimensions if further-neighbor interactions within the layer are included.

Before going on to treat the two-dimensional case, consider briefly the calculation of long-range order, that is, of the spontaneous magnetization $\langle \sigma^{\sigma} \rangle$.

For a completely cyclic system the expectation value of the magnetization is zero, since (using the representation of σ^{z} in terms of n^{\pm}) one has

$$\langle \underline{\sigma}^{\boldsymbol{s}} \rangle = \frac{1}{2} \left[\langle \lambda_0(+) | \underline{\sigma}^{\boldsymbol{s}} | \lambda_0(+) \rangle + \langle \lambda_0(-) | \underline{\sigma}^{\boldsymbol{s}} | \lambda_0(-) \rangle \right] \equiv 0 \quad .$$

$$(3.19)$$

However, as h tends to zero from above

$$\langle \underline{\sigma}^{\sigma} \rangle = \lim_{h \to 0} \langle \lambda_0(+) | \underline{\sigma}^{\sigma} | \lambda_0(+) \rangle \neq 0 \quad . \tag{3.20}$$

Furthermore, with end walls, one may assign any desired configurational weights $W_1(0, \pm)$ and $W_{L+1}(0, \pm)$ to the first and last layers, respective-ly.¹⁰ The spontaneous magnetization is then found to be

$$\langle \underline{\sigma}^{\sigma} \rangle = \langle \lambda_0(+) | \underline{\sigma}^{\sigma} | \lambda_0(+) \rangle$$

$$\times \frac{W_1(0,+)W_{L+1}(0,+) - W_1(0,-)W_{L+1}(0,-)}{W_1(0,+)W_{L+1}(0,+) + W_1(0,-)W_{L+1}(0,-)} , \quad (3.21)$$

where (3.19) has been used. Thus, while $\langle \underline{\sigma}^{z} \rangle \equiv 0$ for a cyclic system, the use of either an infinitesimal field or "free-edge" boundary conditions can lead to nonzero order. It is to be emphasized that this nonzero order in the absence of the field arises from the degeneracy of $\lambda_0(+)$ and $\lambda_0(-)$ in zero field. Note that a *general*-pair-correlation function for the case $(d \ge 3, h \rightarrow 0^*)$ is determined by matrix elements between the zero-particle and single-particle states, so that the decay of any correlation function will be OZ.

D. Decay of Correlation in the Two-Dimensional Zero-Field Ising Model

This section treats the decay of correlation in zero field for the two-dimensional Ising model. Just as in three or more dimensions, there are two noninteracting spectra. Before calculating the decay of correlation, one needs to obtain the effect of $\sigma_{-}^{x}(x)$ acting upon the symmetrical and antisymmetrical eigenstates of <u>K</u>.

First, note that

$$\underline{\sigma}^{\mathbf{r}}(r) | \Phi(A) \rangle = | \Phi(S) \rangle, \quad \underline{\sigma}^{\mathbf{r}}(r) | \Phi(S) \rangle = | \Phi(A) \rangle \quad .$$
(3.22)

The effect of $\underline{\sigma}^{\mathbf{z}}(r)$ and of $\underline{\sigma}^{\mathbf{z}}(r)\underline{\sigma}^{\mathbf{z}}(r+1)$ upon the two-particle states is also needed. For $\sigma^{\mathbf{z}}(r)$,

$$\underline{\sigma}^{\mathbf{z}}(r) | r_1, r_2; A \rangle = (-1)^{\rho(r_1, r_2; r)} | r_1, r_2; S \rangle , \quad (3.23)$$

$$\underline{\sigma}^{z}(r) | r_{1}, r_{2}: S \rangle = (-1)^{\rho(r_{1}, r_{2}; r)} | r_{1}, r_{2}: A \rangle \quad , \quad (3.24)$$

where

$$(-1)^{\rho(r_1,r_2;r)} = -1$$
 for $r_1 < r < r_2$
=+1 otherwise . (3.25)

For $\sigma^{\mathbf{z}}(\mathbf{r})\sigma^{\mathbf{z}}(\mathbf{r}+1)$ one obtains

$$\frac{\sigma^{z}(r)\sigma^{z}(r+1)|x_{1},x_{2}:P\rangle}{=(1-2[\delta(r,x_{1})+\delta(r,x_{2})])|x_{1},x_{2}:P\rangle} \quad (3.26)$$

Therefore, the matrix elements of $\underline{\sigma}^{z}(r)$ are only nonzero between states of opposite parity; and matrix elements involving $\underline{\sigma}^{z}(r)\underline{\sigma}^{z}(r+1)$ are only nonzero between states of like parity; and it follows that the asymptotic decay of $G_{s}(\vec{\mathbf{R}}, 0)$ and $G_{\epsilon}_{-}(\vec{\mathbf{R}}, 0)$ are given by

$$G_{s}(\vec{\mathbf{R}}, \mathbf{0}) \approx \frac{1}{2} \sum_{q_{1}, q_{2}} \exp\left[-\left|r_{\parallel}\right| \hat{\kappa}(q_{1}, q_{2})\right] [\langle \lambda_{0} : S | \underline{\sigma}^{z}(r) \\ \times |\lambda_{2}(q_{1}, q_{2}) : A \rangle \langle \lambda_{2}(q_{1}, q_{2}) : A | \underline{\sigma}^{z}(r) | \lambda_{0} : S \rangle + \langle \lambda : A | \underline{\sigma}^{z}(r) \\ \times |\lambda_{2}(q_{1}, q_{2}) : S \rangle \langle \lambda_{2}(q_{1}, q_{2}) : S | \underline{\sigma}^{z}(r) | \lambda_{0} : A \rangle] \quad (3.27)$$
and

$$G_{\varepsilon_{\perp}}(\vec{\mathbf{R}}, \mathbf{0}) \approx \frac{1}{2} \sum_{P} \sum_{q_{1}, q_{2}} J_{\perp}^{2} \exp[-|r_{\parallel}|\hat{\kappa}(q_{1}, q_{2})]$$

$$\times \langle \lambda_{0} : P | \underline{\sigma}^{\varepsilon}(r) \underline{\sigma}^{\varepsilon}(r+1) | \lambda_{2}(q_{1}, q_{2}) : P \rangle$$

$$\times \langle \lambda_{2}(q_{1}, q_{2}) : P | \underline{\sigma}^{\varepsilon}(r) \underline{\sigma}^{\varepsilon}(r+1) | \lambda_{0} : P \rangle \quad .$$

$$(3.28)$$

In (3. 27) and (3. 28) the difference between the allowed values of q_i for differing parity has been ignored, since this difference is negligible as N tends to infinity. $\hat{\kappa}(q_1, q_2)$ is given by (2.85). Further, (3. 27) and (3. 28) only treat correlation in the layering direction, that is, only for $\vec{R} = r_{\parallel} \hat{z}$.

Equations (2.76) and (2.84) determine the eigenstates (3.27) and (3.28). These together with (3.22)-(3.26) for the action of $\underline{\sigma}^{x}(r)$ on these states determine the matrix elements. These matrix elements have the same character as those for the energy density at high temperatures and zero field; in addition $\hat{\kappa}(q_1, q_2)$ has the form $\hat{\kappa}(q_1) + \hat{\kappa}(q_2)$ as for the two-particle band at high temperatures. The correlation functions are written (as $N \rightarrow \infty$)

$$G_{s}(\vec{\mathbf{R}}, 0) \approx \frac{16u_{\parallel}^{2}e^{-4K_{\perp}}e^{-4K_{\perp}|r_{\parallel}|}}{(1 - e^{-4K_{\perp}})^{2}} \times \int_{-\pi}^{\pi} \frac{dQ}{2\pi} \int_{-\pi}^{\pi} \frac{dq}{2\pi} \sin^{2}q \exp(4u_{\parallel}|r_{\parallel}| \cos\frac{1}{2}Q\cos q)$$
(3.29)

and

$$G_{e_{\perp}}(\vec{\mathbf{R}}, \mathbf{0}) \approx \frac{32 J_{1}^{2} u_{\parallel}^{2} e^{-4K_{\perp}} e^{-4K_{\perp}|\mathbf{r}_{\parallel}|}}{(1 - e^{-4K_{\perp}})^{2}} \\ \times \int_{-\pi}^{\pi} \frac{dQ}{2\pi} \int_{-\pi}^{\pi} \sin^{2}q \exp(4u_{\parallel}|\mathbf{r}_{\parallel}| \cos\frac{1}{2}Q \cos q) \quad .$$
(3.30)

These are exactly the forms displayed in Eq. (5.16) of Paper II² (with d=2), so that the asymtotic analysis presented in the Appendix of that paper may be taken over directly to analyze (3.29) and (3.30). The results are

$$G_{s}(\vec{\mathbf{R}}, \mathbf{0}) \approx \frac{2u_{\parallel}^{2} e^{-4K_{\perp}}}{(1 - e^{-4K_{\perp}})^{2}} \frac{e^{-\kappa R}}{(u_{\parallel}R)^{2}}$$
(3.31)

and

$$G_{e_{\perp}}(\vec{\mathbf{R}}, 0) \approx \frac{4u_{\parallel}^2 e^{-4K_{\perp}} J_{\perp}^2}{(1 - e^{-4K_{\perp}})^2} \frac{e^{-\kappa R}}{(u_{\parallel} R)^2} , \qquad (3.32)$$

where $R = |r_{\parallel}|$ and κ is given by the $q_1 = q_2 = 0$ limit of Eq. (2.85), namely, by

$$\kappa = 4(K_1 - u_0) + O(u_0^2) \quad . \tag{3.33}$$

These results are in agreement with the results of Kadanoff⁴ and of Cheng and Wu¹¹ for the decay of spin correlation functions, and agree with the results found by Stephenson¹² and by Hecht¹³ for the four-spin or energy-density correlation functions. Neither (3.31) nor (3.32) exhibits OZ behavior. Further, a short calculation shows that the threespin function $\langle \delta S^{r}(0) \delta \epsilon_{\perp}(r_{\parallel}) \rangle$, which is identically zero in the completely cyclic case, decays as

$$R^{-2}e^{-\kappa R} \tag{3.34}$$

in the case of end walls. One may fully expect that for this system *all* nonzero *pair* correlation functions decay as (3.34) since the matrix elements for any correlation function between zero and two-particle states are finite.

IV. SUMMARY

It has been found that at low temperatures—except for the d=2, h=0 model with nearest-neighbor forces—the decay of correlation in the Ising model verifies the OZ prediction¹:

$$G_{AB}(R, h, d) \approx D_{AB}(d, h) e^{-\kappa R} / R^{(d-1)/2}$$
 (4.1)

For the special case of the d=2, h=0 model with nearest-neighbor forces the OZ form is replaced by

$$G_{AB}(R, h=0, d=2) \approx D_{AB} e^{-\kappa R}/R^2$$
 (4.2)

The difference between the general case and the d=2, h=0 case arises because in the general case the decay of correlation is determined by the largest level and the single-particle states of the transfer matrix, but in the special case the single-particle states are replaced by two-particle states.

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Dynamics of Localized Magnetic Moments in Metals in the Presence of the Electron-Electron Interaction*

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Using the Feynman-diagram technique and the Abrikosov fermion representation for the localized moment, the transverse dynamic susceptibility of a dilute alloy is derived in the presence of the electron-electron interaction. In the paramagentic region, enhancement factors for the Overhauser and Korringa rates are found to contain identical averages over the wave vectors \vec{q} spanning the Fermi surface. The former is also deenhanced by the inverse of the uniform magnetization enhancement factor $1-V_0\rho$ arising from the relaxation to the self-consistently enhanced instantaneous local field. The exchange-enhanced detailed-balance condition follows immediately. Our theory represents the first microscopic derivation of this relation between the enhanced relaxation rates and the static electron-electron-enhanced susceptibilities.

I. INTRODUCTION

Recently, Barnes and Zitkova-Wilcox¹ (BZ) derived a pair of coupled linear equations describing the electron-spin resonance in a dilute alloy. In the classical regime and for equal g factors, these equations are comparable to those of Hasegawa's case B.² The BZ treatment did not include the Coulomb interaction between the conduction electrons, however, which is known to enhance³ the local-moment g shift Δg_s and the local-moment (Korringa) relaxation rate $1/T_{se}$.⁴ The coupled resonance in the presence of this (exchange) enhancement is ordinarily assumed to be described by the usual Bloch equations in the form displayed by Cottet et al.⁵ However, there exists no satisfactory microscopic derivation of the electronic relaxation rate due to the local-moment-conduction-electron interaction for the interacting electron gas. Recent electron-spin-resonance studies⁶ in $Gd_xLa_{1-x}Al_2$ intermetallic compounds were analyzed using the so-called detailed-balance condition, i.e., the relation between the static localized and conduction-electron susceptibilities and the Korringa and Overhauser rates in the presence of the electron-electron interaction. In analogy with the spin-orbit scattering, 7 one can argue that in the presence of the electron exchange enhancement also the effective s-d scattering cross section goes to zero proportional to the inverse static susceptibility as the ferromagnetic limit is approached. However, if one tries to modify the ordinary Overhauser rate accordingly, [e.g., by the Brinkman and Engelsberg factor $(1 - \vec{I})^7$] one arrives at values of $1/T_{\rm es}$, which violate the mathematical equality of the detailed-balance relation.

The purpose of this paper is to investigate in a systematic way the effect of the electron-electron interaction on the coupled susceptibility. We will