=0.150 b, which agrees with the value quoted in Ref. 1, as expected. However, if one includes also the local contributions from $2p$ and $3d$ orbitals of Fe^{3+} the value of Q is further lowered.

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Behavior of Two-Point Correlation Functions Near and on a Phase Boundary*

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The asymptotic decay of the two-point correlation function $G_{AB}(\vec{R})$ at and near a phase-separation point is discussed for d-dimensional, spin-$\frac{1}{2}$ Ising models at low temperature. The general behavior, even on the phase boundary ($H=0$), is in agreement with extended Ornstein-Zernike predictions. It is shown why the nearest-neighbor two-dimensional model in zero field is an exception. The decay of $G_{AB}(\vec{R}_1, \vec{R}_2)$ near a free surface at high temperatures agrees with phenomenological predictions using a vanishing boundary condition. At low temperature, however, the decay of correlation near a surface is exponentially slower than in the bulk.

The great utility of the Ornstein-Zernike (O-Z) and Landau-type phenomenological theories for discussing fluctuations in condensed systems is well recognized. Although these approaches generally break down in the immediate vicinity of a critical point,[1-3] the familiar prediction that the correlation function

$$G_{AB}(\vec{R}_1;\vec{R}) = \langle \hat{A}(\vec{R}_1)\hat{B}(\vec{R}_1+\vec{R})\rangle - \langle \hat{A}(\vec{R}_1)\rangle\langle \hat{B}(\vec{R}_1+\vec{R})\rangle \tag{1}$$

should decay as $e^{-\kappa R}/R^{(d-1)/2}$ as $R\to\infty$ (when $\vec{R}_1$ is far from any surfaces) is believed to be of much wider generality, at least when the operators $\hat{A}$ and $\hat{B}$ are both identified as the relevant order parameter $\hat{\Psi}$. In an earlier note[4] we examined this general O-Z hypothesis at high temperatures (considering specifically spin-$\frac{1}{2}$, d-dimensional Ising models) and demonstrated that as $R\to\infty$,

$$G_{AB}(\vec{R}_1;\vec{R}) \approx D_A^{(1)}D_B^{(1)}(e^{-\kappa R}/R^{(d-1)/2})[1+O(R^{-1})] + D_A^{(2)}D_B^{(2)}(e^{-\kappa_{ii} R}/R^{d})[1+O(R^{-1})]+\cdots, \tag{2}$$

where the inverse correlation range $\kappa = \frac{1}{2}\kappa_{ii}$ and the amplitudes $D_A^{(1)}$, etc., are dependent upon T and upon the ordering field ζ ($\equiv H$). The O-Z prediction is thus confirmed, in general, although for certain operators (containing, like the energy $\mathcal{E}$, only products of even numbers of spins) the leading "single-particle" amplitudes $D_A^{(1)}$ vanish in zero field ($H\equiv 0$), leaving the second-order or "two-particle" term as the dominant decay law.

Nevertheless doubt is cast on the general validity of the extended O-Z prediction by the exact results[5] for the two-dimensional nearest-neighbor spin-$\frac{1}{2}$ Ising models in zero field below the critical point T_c (i.e., on the phase boundary). Here the spin-spin ($G_{\Psi\Psi}$), spin-energy ($G_{\Psi\mathcal{E}}$), and energy-energy ($G_{\mathcal{E}\mathcal{E}}$) correlation functions *all* decay as $e^{-\kappa R}/R^2$ (in place of the expected $e^{-\kappa R}/R^{1/2}$).[5] The spin-inversion symmetry is broken for all $T<T_c$ and there is no obvious reason why all the amplitudes $D^{(1)}$ should vanish [although the remaining two-particle term in (2) would then have the correct form].

In the present note, we report on a study of d-dimensional ferromagnetic spin-$\frac{1}{2}$ Ising models at *low* temperatures which answers these doubts. We show (A) that when $H\neq 0$ (i.e., "near" the phase boundary), the leading decay is always of O-Z or "single-particle" form with, however, (B) dominant corrections of the *same* form but different range parameter κ_{ii} ($\kappa<\kappa_{ii}<2\kappa$) rather than of the "two-particle" form exhibited in (2); (C) the conclusions (A) and (B) remain valid on the phase boundary, $H=0$, for all cases *except* (D) the $d=2$ nearest-neighbor Ising models where the exact results[5] are reproduced by a "two-particle" decay law; if second-neighbor interactions are introduced, the O-Z decay law is restored.[6]

As a further, more sensitive test of the general O-Z hypothesis, we have also studied the decay of correlation *near a surface*. A surface or edge of dimensionality $d_\parallel$ ($=1, 2, \cdots, d$) is defined by the incidence of $d_\perp = d - d_\parallel$ "planar" $(d-1)$-dimensional boundary "surfaces."[7] If x_α and y_α are the respective distances of the points $\vec{R}_1$ and $\vec{R}_2 = \vec{R}_1 - \vec{R}$ from the αth bounding surface ($\alpha = 1, 2, \cdots, d-1$), we find

$$G_{AB}(\vec{R}_1, \vec{R}) \approx D_A{}^\times D_B{}^\times F(x_1 \cdots y_{d_\perp}; R) e^{-\kappa^\times R}/R^\Psi \tag{3}$$

with $F(R) \to$ const as $R \to \infty$; the superscript $\times$ denotes boundary properties. Then, (E) at *high temperatures,* as considered in I,[4] we obtain

$$\kappa^\times(H, T) \approx \kappa(H, T), \quad \Psi(d, d_\perp) = \tfrac{1}{2}(d-1) + d_\perp, \tag{4}$$

so that the surface correlation range is the *same* as the bulk range although the decay is more rapid by factor $R^{-d_\perp}$. In addition, one finds $F = \prod_\alpha f(x_\alpha, y_\alpha; R)$, and $D_A{}^\times = D_A{}^{(1)}$, with

$$f(x, y; R) \approx R\{1 - \exp[-(x+a)(y+a)/\epsilon R]\} \tag{5}$$

for $x/R, y/R \ll 1$, where a is the lattice spacing, and[4] $\epsilon(H, T)$ may be related to the angular variation of $\kappa(H, T)$ [see also Eq. (9) below]. From (5) one can see how the bulk O-Z behavior is restored as x_α and y_α become large. These results confirm in detail the predictions of the phenomenological theories[8] if the usual partial differential equation for $\Psi(\vec{R})$ is solved (using, say, the method of images) with the boundary condition $\Psi(\vec{R}) \equiv 0$ for $\vec{R}$ on the surface which, microscopically, is to be taken one lattice layer *outside* the layer of surface spins. On the other hand, (F) at *low temperatures and for all H* we find

$$\kappa^\times(H, T) \simeq \kappa - d_\perp(2J/k_BTa) < \kappa(H, T), \tag{6}$$

$$\Psi(d, d_\perp) = \tfrac{1}{2}(d_\parallel - 1) = \tfrac{1}{2}(d - d_\perp - 1), \tag{7}$$

where J is the spin-spin coupling energy, so that the decay near a surface is *exponentially slower* than in the bulk; the exponent Ψ is also smaller. However one finds that the amplitude factor F in (3) varies as $e^{-\kappa^*(x+y)}$ with $\kappa^* \sim J/k_BT$, which means that the surface contribution to G_{AB} rapidly damps out as x_α and y_α increase, leaving only the more rapidly decaying terms like (3) with (4). These special surface effects are *not* predicted by the usual phenomenological theories. Finally, (G) the *nearest-neighbor two-dimensional lattice in zero field* is again a special case with $\kappa^\times \simeq \frac{1}{2}\kappa$ but with $\Psi = 1\frac{1}{2}$ for $d_\parallel = d_\perp = 1$, rather than zero as predicted by (7).

The conclusions (A)-(G) above are based on detailed calculations using the transfer-matrix approach[4,9] for ferromagnetic Ising systems in a field H ($=k_BTL$) with nearest-neighbor interactions J' ($=k_BTK'$) between spins in adjacent $(d-1)$-dimensional "layers" of N spins,[4] and with interactions J ($=k_BTK$) between spins within each layer.[6] A low-T perturbation theory is developed by writing the transfer matrix as[10]

$$\vec{K} = \vec{K}_0[\vec{1} + w\vec{V}_1 + w^2\vec{V}_2 + \cdots], \quad w = e^{-2K'}, \tag{8}$$

where $\vec{K}_0$ is diagonal in the representation of the eigenstates of a layer. As in I we may write the eigenvalues as $\lambda_j = \exp(-aE_j)$ and interpret the $E_j(H, T)$ as energy levels of a many-body system. In *zeroth order* when $H > 0$ the vacuum state $|0\rangle$ is given by all spins "up," while "particles" correspond merely to "overturned" spins. The higher states, in order of increasing excitation energy ω, are the following for periodic boundary conditions: (i) N localized single-particle states with $\omega_i{}^{(0)}a = 4(d-1)K + 2L$; (ii) $(d-1)N$ bound-pair states of two adjacent particles with $\omega_{ii}{}^{(0)}a = 2\omega_i{}^{(0)}a - 4K$; (iii) $\frac{1}{2}N(N-2d+1)$ unbound-pair states of two non-neighboring particles with $\omega_{iii}{}^{(0)} = 2\omega_{ii}{}^{(0)}$; and so on. In second order the perturbations split the degeneracies (and mix in states of other particle number) leading, as in I, to a lowest band of single-particle states $|\vec{q}\rangle$, of excitation energy

$$\omega_i(\vec{q}) = \kappa(H, T) + \epsilon(H, T)q^2 + O(q^4), \tag{9}$$

where $\vec{q}$ is a wave vector of dimensionality $d-1$ and

$$\kappa a = 4(d-1)K + 2L + w^2[1 - 4(d-1)Y_{d-2} + 2(2d-1)Y_{d-1}] + O(w^4), \tag{10}$$

$$\epsilon = a[Y_{d-2} - Y_{d-1}]e^{-4K'} + O(w^4), \tag{11}$$

with

$$Y_n(H, T) = (e^{4nK+2L} - 1)^{-1}. \tag{12}$$

The bound-pair states likewise yield a single-particle band $\omega_{ii}(\vec{q})$ with gap $\kappa_{ii}a \simeq \kappa a + 4K > \kappa a$, while the unbound-pair states yield a two-particle band $\omega_{iii}(\vec{q}, \vec{q}\,')$ with $\kappa_{iii} \simeq 2\kappa > \kappa_{ii}$. The asymptotic decay of $G_{AB}(\vec{R}_1, \vec{R})$ for large $\vec{R}$ now follows,[11] as in I, from a knowledge of the matrix elements[4] between the states $|0\rangle$ and $|\vec{q}\rangle$ for which we find, in leading order,

$$M_A{}^{(i)}(\vec{q}) \propto w/|\sinh[2(d-1)K + L]| \propto D_A{}^{(i)}. \tag{13}$$

Since for general $\hat{A}$ (including spin and energy operators) these are nonvanishing for small q, the previous arguments[4] lead directly to the O-Z form [first term in (2)]. The second band of excited states also has a single-particle character and so the next group of corrections are again of O-Z form but with κ_{ii} replacing κ. These arguments establish conclusions (A) and (B).

In zero field the spectrum of $\vec{K}_0$ is doubled up as there are two vacuum states $|0^+\rangle$ and $|0^-\rangle$ (all spins "up," and all "down"). However the two spectra mix only in order $\propto N$, and thus the previous calculations stand if one lets H (and L) $\to 0$, so confirming (C) provided $d > 2$. In two dimensions one cannot allow $H \to 0$ since in (10) and (11) one has $Y_{d-2}(H) \sim H^{-1} \to \infty$. This arises physically because the zeroth-order zero-field single-particle and bound-pair states are degenerate when $d = 2$. Furthermore these states are also degenerate with bound triplets, bound quadruplets, $\cdots$, corresponding to "domains" of $3, 4, \cdots$ adjacent overturned spins on a linear Ising chain. To classify this lowest band of $N(N-1)$ excited states one can label the positions x and y of the ends of the "domain": This yields a two-particle band except that "particles" must now be understood as *interfaces* or domain-wall points. This band splits in first order, giving

$$\omega_i(q, q'^1) = \kappa(T) + \epsilon(T)(q^2 + q'^2) + O(q^4, q'^4, q^2 q'^2), \tag{14}$$

with

$$\kappa a = 4K - 4w + O(w^2), \quad \epsilon = a e^{-2K'} + O(w^2). \tag{15}$$

Owing to the obvious "hard-core" condition $x \neq y$, the two-particle wave function has the form

$$\langle x, y | q, q' \rangle = N^{-1}\sqrt{2}\, \exp[i(q + q')(x + y)/2] \sin[\tfrac{1}{2}(q - q')(x - y)]. \tag{16}$$

This introduces a factor $\sin\frac{1}{2}(q-q') \sim (q-q')$ into all the matrix elements $M_A{}^{(i)}(q, q')$ which, on evaluating the integrals[4] for $G_{AB}(\vec{R})$ for large R, leads directly to the form $e^{-\kappa R}/R^2$ as stated in (D) [compare with I and the second term in (2)]. The value of κ and the amplitudes D_A obtained agree with the exact results[5] to the appropriate order in w. The introduction of, say, second-neighbor ferromagnetic interactions is easily seen to stabilize the single overturned spins relative to the domain states. The form (2), with leading O-Z behavior, is thus regained with $\kappa_{ii}a \simeq \kappa a + (4J_2/k_B T)$.

By derivation, our results are valid for low T and general H. However, we expect the dominant O-Z behavior to remain valid as $R \to \infty$ at fixed T and $H \neq 0$ even in the critical region. In zero field, however, the "anomalous" decay found in the nearest-neighbor $d = 2$ Ising model may well take over more generally as $T \to T_c$. As we have demonstrated, this mode of decay is intimately connected with the "diffusion" of the interface, or domain wall, between regions of coexisting conjugate phases. As such it might be a dominant fluctuation and correlation mechanism near the critical point in two and three dimensions.[12]

Finally, to establish the results (E)-(G) for decay near a surface, the same approach suffices. At high T the main effect of a surface is to replace a factor e^{iqx} in the single-particle wave function by a factor $\sin q(x + a)$; the spectrum does not change significantly. This sine factor enters the matrix elements $M_A{}^{(1)}(q)$ and thence yields the factor $f(x, y; R)$ of (5) with Ψ given by (4). At low T, spins overturned on the surface have a lower energy than the bulk single-particle states by $2J/k_B Ta$ for each exposed face. These states lead to a surface band of dimensionality $d_\parallel$ with gap (6), and, hence, corresponding O-Z behavior with d replaced by $d_\parallel$ as in (7). The lowest states for the $d = 2$ nearest-neighbor case when $H = 0$ are again exceptional, being a set of $N-1$ single interfaces (i.e., all spins overturned for $r > x$) with $\kappa^\times a \approx 2K \approx \frac{1}{2}\kappa a$. The analysis is then similar to that for the single-particle band at high T, with the corresponding result that $\Psi = \frac{1}{2}(d-1) + d_\parallel = 1\frac{1}{2}$. However the matrix elements of local operators $\hat{A}$ between these states and $|0^\pm\rangle$ decay exponentially with distance from the surface.

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[6]We have considered explicitly the two-dimensional square Ising model with ferromagnetic second-neighbor interactions in the layers perpendicular to the direction $\vec{R}$.

[7]We consider d-dimensional hypercubic lattices with surfaces perpendicular to the cubic axes. When $d=3$ the case $(d_\perp=1, d_\parallel=2)$ describes correlations near a single planar surface; $(d_\perp=2, d_\parallel=1)$ means that both $\vec{R}_1$ and $\vec{R}_2$ lie near the intersection of two plane surfaces, that is, near a one-dimensional edge of the simple cubic lattice. Note that $d_\perp=0$ always implies the bulk situation.

[8]To our knowledge these phenomenological predictions have not previously been reported.

[9]For further references see I.

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[11]As in I we assume $\vec{R}$ lies in a direction close to the axis along which the lattice is built up. The perturbation theory generates successive angular corrections.

[12]We may also recall that the interfacial tension vanishes as $T \to T_c$, thus enhancing such fluctuations (see also Ref. 10).

Diffraction Systematics of Nuclear and Particle Scattering

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It is shown that, contrary to popular belief, diffraction scattering in nuclear and particle physics is not always of Fraunhofer type. By establishing a simple physical connection between scattering in a Coulomb field and Fresnel diffraction we show that diffractive collisions of heavy charged particles are predominantly of Fresnel type. We derive quantitative criteria for Fraunhofer and Fresnel scattering which lead to a new classification of all scattering processes.

Diffraction effects in nuclear and particle scattering have been known for a long time and are believed to be well understood. At high enough energy, elastic scattering can be regarded as shadow scattering in the presence of a large number of nonelastic processes; thus diffraction is a consequence of the unitarity of the scattering matrix. It is commonly assumed that all diffraction scattering is of Fraunhofer type. The argument is simple[1]: In all nuclear scattering situations the particle source and the point of observation are practically at "infinity" relative to the dimensions of the scattering object. If the energy is high enough such that the wavelength is small compared to the radius of the interaction region, it seems obvious that we have the conditions for Fraunhofer diffraction.

However, several years ago it was noticed[2] that well-known features in the angular distributions for scattering of complex nuclei closely resemble the characteristics of Fresnel diffraction in optics. It was shown that these "Fresnel effects" are associated with the Coulomb interaction. In a certain well-defined limit, which corresponds to high energy and a strong Coulomb field, the analytic expression in the strong-absorption model[3] for the ratio of the differential scattering cross section $\sigma(\theta)$ to the Rutherford cross section $\sigma_R(\theta)$ reduces to the simple formula

$$\sigma(\theta)/\sigma_R(\theta) = \tfrac{1}{2}\{[\tfrac{1}{2}-C(w)]^2 + [\tfrac{1}{2}-S(w)]^2\}, \qquad (1)$$

where $C(w)$ and $S(w)$ are the Fresnel integrals