

Critical Behavior of Magnets with Dipolar Interactions. III. Antiferromagnets

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Exact renormalization group recursion formulas, derived in Paper I for $\epsilon = 4 - d$ small, are applied to antiferromagnets. It is shown, that in contrast to the ferromagnetic case, the main parameters characterizing the dipolar interactions become irrelevant for antiferromagnets, so that the critical exponents maintain their short-range values. However, the relative decay of the dipolar parameters is slow (the appropriate exponents being of order ϵ^2), and thus the possibility of observing their existence experimentally is discussed briefly. In addition, the dipolar anisotropies, deriving from the lattice structure, produce weak instabilities which are even harder to detect than in the ferromagnetic case. Ferromagnetic short-range anisotropy is considered briefly. The Appendix contains a calculation of the renormalization group eigenvalues of the operators $\sum_{\mathbf{R}} S_{\mathbf{R}}^4$ and $\sum_{\mathbf{R}} (S_{\mathbf{R}}^4)^4$. The latter is shown to be relevant.

I. INTRODUCTION

In two previous papers^{1,2} [hereafter referred to as I (Ref. 1) and II (Ref. 2)], the critical behavior of ferromagnets, with dipolar interactions as well as isotropic exchange coupling, was analyzed using renormalization-group and graphical-expansion techniques for dimensionality $d = 4 - \epsilon$ with ϵ small. It was shown, that close to the critical temperature a characteristic isotropic dipolar behavior appears, with a special angular dependence of the correlation functions, and with new critical exponents. These results were based on an analysis of the behavior of the various terms appearing in the Fourier transform of the dipolar interactions.

In a paper³ summarizing this analysis, we argued that the dipolar results should be relevant to various ferromagnets, such as the europium chalcogenides, which had previously been considered well characterized by pure short-range Heisenberg coupling.

Recent heat-capacity experiments⁴ on RbMnF₃ and EuO indicate, that the critical behavior of antiferromagnets may be significantly different from that of otherwise comparable ferromagnets. Since the ferromagnet's behavior is modified by dipolar forces, it is interesting to investigate the effects of dipolar interactions on antiferromagnets. This is the problem treated in the present paper.

In Sec. II we discuss the appropriate Hamiltonian, and emphasize the differences between ferromagnets and antiferromagnets. The main difference arises simply because in antiferromagnets the important region of momentum space is not the origin, but rather the corner of the Brillouin zone, where the nonanalytic part of the Fourier transform of the dipolar interaction is not present.

Section III contains a reformulation of the exact renormalization-group recursion relations, and a discussion of the irrelevance of the dipolar param-

eters. The fixed points and the critical behavior of the system are studied in Sec. IV. Section V includes a discussion of the results, mentioning possible extensions and briefly reviewing the experimental situation. The Appendix considers the anisotropic (lattice) instabilities, which govern the behavior of the system very close to T_c (and beyond present experimental resolution).

II. HAMILTONIAN

The Hamiltonian of an antiferromagnet with isotropic exchange coupling and dipolar interactions may be written

$$\mathcal{H} = -\frac{1}{2} \sum_{\mathbf{R} \neq \mathbf{R}'} J(\mathbf{R} - \mathbf{R}') \vec{S}_{\mathbf{R}} \cdot \vec{S}_{\mathbf{R}'} - G \sum_{\mathbf{R} \neq \mathbf{R}'} \sum_{\alpha\beta} \frac{\partial^2}{\partial R^\alpha \partial R'^\beta} \times \left(\frac{1}{|\mathbf{R} - \mathbf{R}'|^{d-2}} \right) S_{\mathbf{R}}^\alpha S_{\mathbf{R}'}^\beta, \quad (1)$$

where $J(\mathbf{R})$ will be negative at nearest-neighbor positions and significantly smaller in magnitude at larger distances (see below). All other quantities are defined as for the ferromagnet (see Paper I): $\vec{S}_{\mathbf{R}}$ is a d -component spin; $G = \frac{1}{2}(g\mu_B)^2$, where g is the gyromagnetic ratio per ion and μ_B is the Bohr magneton.

Since we expect the spins to order on two sublattices, with opposite directions, we shall modify the definition of the Fourier-transformed spin variables used in I and II. Let \vec{k}_0 be a reciprocal-lattice vector, such that $e^{i\vec{k}_0 \cdot \mathbf{R}}$ has opposite signs on the lattice points of the two sublattices. For a d -dimensional simple cubic lattice with a lattice spacing a , $k_0^\alpha = \pi/a$ is such a vector. We consider only bipartite lattices, for which \vec{k}_0 can always be similarly defined. The transformed spin variables $\sigma_{\vec{q}}^\alpha$ are then defined by

$$\sigma_{\vec{q}}^\alpha = \sum_{\mathbf{R}} e^{i(\vec{q} + \vec{k}_0) \cdot \mathbf{R}} S_{\mathbf{R}}^\alpha. \quad (2)$$

Since $S_{\vec{R}}^\alpha$ is real, and since $e^{i\vec{k}_0 \cdot \vec{R}} = \pm 1$, it is straightforward to show that

$$(\sigma_{\vec{q}}^\alpha)^* = \sigma_{-\vec{q}}^\alpha. \quad (3)$$

The correlation function of two spins will be of the form

$$\begin{aligned} \langle S_{\vec{R}}^\alpha S_0^\beta \rangle &= \int_{\vec{q}} \int_{\vec{q}'} e^{-i\vec{R} \cdot (\vec{q} + \vec{q}')} \langle \sigma_{\vec{q}}^\alpha \sigma_{\vec{q}'}^\beta \rangle \\ &= e^{-i\vec{R} \cdot \vec{k}_0} \int_{\vec{q}} e^{-i\vec{R} \cdot \vec{q}} \Gamma^{\alpha\beta}(\vec{q}), \end{aligned} \quad (4)$$

where $\int_{\vec{q}}$ denotes $(2\pi)^{-d}$ times the integral over the first Brillouin zone, and where

$$\Gamma^{\alpha\beta}(\vec{q}) = \langle \sigma_{\vec{q}}^\alpha \sigma_{\vec{q}'}^\beta \rangle / \delta(\vec{q} + \vec{q}'). \quad (5)$$

The factor $e^{-i\vec{R} \cdot \vec{k}_0}$ thus represents the fact that the two sublattices will order with opposite spin orientation.

Rewriting (1) in terms of the $\sigma_{\vec{q}}^\alpha$ leads to

$$\begin{aligned} \mathcal{K} &= -\frac{1}{2} \sum_{\alpha} \int_{\vec{q}} \hat{J}(\vec{k}_0 + \vec{q}) \sigma_{\vec{q}}^\alpha \sigma_{-\vec{q}}^\alpha \\ &\quad + Ga^{-d} \sum_{\alpha\beta} \int_{\vec{q}} A^{\alpha\beta}(\vec{k}_0 + \vec{q}) \sigma_{\vec{q}}^\alpha \sigma_{-\vec{q}}^\beta, \end{aligned} \quad (6)$$

where the integral is over $|\vec{q}| < \pi$ and

$$\hat{J}(\vec{k}) = \sum_{\vec{R}} e^{i\vec{k} \cdot \vec{R}} J(\vec{R}) \quad (7)$$

and

$$A^{\alpha\beta}(\vec{k}) = -a^d \frac{\partial^2}{\partial R^\alpha \partial R^\beta} \left(\sum_{\vec{R}_1} \frac{e^{i\vec{k} \cdot \vec{R}_1}}{|\vec{R}_1 - \vec{R}|^{d-2}} \right)_{\vec{R}=0}. \quad (8)$$

[The summation in Eq. (8) is over all lattice points except $\vec{R}_1 = 0$.]

It is easy to show that if $J(\vec{R}) = -|J|$ for the c nearest neighbors but is zero elsewhere, then one has

$$\hat{J}(\vec{k}_0 + \vec{q}) = c|J| \left(1 - \frac{1}{2}d^{-1}q^2 \right) + O(q^4), \quad (9)$$

where for convenience we have taken units in which $a=1$. More generally, we may replace $c|J|$ in this expression by $\hat{J}(\vec{k}_0)$, which should still be positive, and by expanding in powers of q^2 , replace $\frac{1}{2}d^{-1}$ by a positive coefficient of similar magnitude.

The Fourier transform of the dipolar forces $A^{\alpha\beta}(\vec{k})$ has been discussed thoroughly in I. A direct symmetry argument shows, that for bipartite Bravais lattices⁵

$$A^{\alpha\beta}(\vec{k}_0) = 0. \quad (10)$$

For simplicity, we shall restrict ourselves at this point to the simple cubic case, postponing consideration of other cubic lattices until Sec. V.

As shown in I, $A^{\alpha\beta}(\vec{k})$ is nonanalytic for $\vec{k} = \vec{q}_h$, where \vec{q}_h is a vector connecting two sites in the re-

ciprocally lattice. Clearly, \vec{k}_0 is not such a vector; hence we may expand $A^{\alpha\beta}(\vec{k})$ in a Taylor series in the vicinity of $\vec{k} = \vec{k}_0$. As might be anticipated, the critical behavior will be governed by the behavior of $J(\vec{k}_0 + \vec{q})$ and of $A^{\alpha\beta}(\vec{k}_0 + \vec{q})$ for small values of \vec{q} , hence we need not worry about the nonanalyticity of $A^{\alpha\beta}$ far from \vec{k}_0 . The integrals on \vec{q} run over a Brillouin zone, namely, $|q^\alpha| \leq \pi/a$ for the simple cubic case. Only at the corners, $k_0^\alpha + q^\alpha = 2\pi/a$ or 0, shall we have a nonanalytic contribution. However, $A^{\alpha\beta}(\vec{k})$ is bounded everywhere, and the contribution of a few points should not affect the values of the integrals.

In the vicinity of k_0 , we can use simple symmetry arguments to show that $A^{\alpha\beta}(\vec{k}_0 + \vec{q})$ has the form

$$\begin{aligned} A^{\alpha\beta}(\vec{k}_0 + \vec{q}) &= \delta_{\alpha\beta} [b_4 q^2 - b_5 (q^\alpha)^2] + b_2 q^\alpha q^\beta \\ &\quad + O((q^\alpha q^\beta)^2, q^4). \end{aligned} \quad (11)$$

In the three-dimensional case, the numerical results of Cohen and Keffer⁶ suggest that b_2 , b_4 and b_5 are positive, and that explains our choice of the signs in (11). The indices were chosen to emphasize the similarity to (9) of I. Using these expressions, (6) becomes

$$\begin{aligned} \mathcal{K} &= \frac{1}{2} \sum_{\alpha\beta} \int_{\vec{q}} \{ [-c|J| + \tilde{J}q^2 - 2Ga^{-d}b_5(q^\alpha)^2] \delta_{\alpha\beta} \\ &\quad + 2Ga^{-d}b_2 q^\alpha q^\beta + O((q^\alpha q^\beta)^2, q^4) \} \sigma_{\vec{q}}^\alpha \sigma_{-\vec{q}}^\beta, \end{aligned} \quad (12)$$

where the integral is over $|\vec{q}| < \pi$ and

$$\tilde{J} = c|J| / (2d) + 2Ga^{-d}b_4. \quad (13)$$

The partition function for the continuous-spin s^4 model is how

$$Z = \int_{\sigma} e^{\mathcal{K}}, \quad (14)$$

with (see Paper I) the reduced Hamiltonian

$$\bar{\mathcal{K}} = -\frac{\tilde{\mathcal{K}}}{kT} - \frac{1}{2} \sum_{\vec{R}} \tilde{S}_{\vec{R}}^2 - u \sum_{\vec{R}} (S_{\vec{R}}^2)^2 - v \sum_{\vec{R}} \sum_{\alpha} (S_{\vec{R}}^\alpha)^4, \quad (15)$$

which may be written

$$\begin{aligned} \bar{\mathcal{K}} &= -\frac{1}{2} \sum_{\alpha\beta} \int_{\vec{q}} \tilde{U}_2^{\alpha\beta}(\vec{q}) \sigma_{\vec{q}}^\alpha \sigma_{-\vec{q}}^\beta - \sum_{\alpha\beta} (u + \delta_{\alpha\beta}v) \\ &\quad \times \int_{\vec{q}_1} \int_{\vec{q}_2} \sigma_{\vec{q}_1}^\alpha \sigma_{\vec{q}_1}^\alpha \sigma_{\vec{q}_2}^\beta \sigma_{-\vec{q}_1 - \vec{q}_2}^\beta, \end{aligned} \quad (16)$$

with

$$\tilde{U}_2^{\alpha\beta}(\vec{q}) = \left(\tilde{r} + \frac{\tilde{J}}{kT} q^2 - 2 \frac{Gb_5}{kTa^d} (q^\alpha)^2 \right) \delta_{\alpha\beta} + 2 \frac{Gb_2}{kTa^d} q^\alpha q^\beta, \quad (17)$$

$$\tilde{r} = 1 - c|J| / kT. \quad (18)$$

In Eq. (16) we have ignored terms of order q^4 , $(q^\alpha q^\beta)^2$, since they turn out to be irrelevant.

As in I, we now suppose the exchange forces are

dominant, in particular,

$$4d|b_4|G/c|J|a^d \gg 1, \quad (19)$$

so that $\bar{J} > 0$. This assumption is, in fact, necessary only if $b_4 < 0$ (for $d=3$, indeed, we have $b_4 > 0^6$). Otherwise, we shall see that our results are valid for any value of the ratio (19), as long as $2Gb_5/\bar{J}a^d \ll 1$. With $\bar{J} > 0$ we may rescale all spins by a factor $(kT/\bar{J}\pi^{d+2})^{1/2}$, leading to

$$\begin{aligned} \bar{\mathcal{H}}_0 = & -\frac{1}{2} \sum_{\alpha\beta} \int_{\vec{q}} U_2^{0,\alpha\beta}(\vec{q}) \sigma_{\vec{q}}^\alpha \sigma_{-\vec{q}}^\beta - \sum_{\alpha\beta} (u_0 + \delta_{\alpha\beta} v_0) \\ & \times \int_{\vec{q}_1} \int_{\vec{q}_2} \sigma_{\vec{q}_1}^\alpha \sigma_{\vec{q}_2}^\alpha \sigma_{-\vec{q}_1-\vec{q}_2}^\beta, \quad (20) \end{aligned}$$

with the \vec{q} integration being over $|\vec{q}| < 1$,

$$U_2^{0,\alpha\beta}(\vec{q}) = [\tau_0 + q^2 - f_0(q^\alpha)^2] \delta_{\alpha\beta} + h_0 q^\alpha q^\beta, \quad (21)$$

$$\tau_0 = \bar{\tau} k T / \bar{J} \pi^2 = k(T - T_0) / \bar{J} \pi^2, \quad k T_0 = c |J|, \quad (22)$$

and

$$\begin{aligned} f_0 = 2Ga^{-d}b_5/\bar{J}, \quad h_0 = 2Ga^{-d}b_2/\bar{J}, \\ u_0 = u(kT/\bar{J})^2\pi^{d-4}, \quad v_0 = v(kT/\bar{J})^2\pi^{d-4}. \quad (23) \end{aligned}$$

Expression (20) is very similar to the corresponding formula [Eq. (16) of I], except for the absence of the nonanalytic dipolar term $q^\alpha q^\beta / q^2$, and for the change in the signs of f_0, h_0 . In the notation of I, this means that $g_0 = 0$. Since it was the dipolar parameter g_0 that led to a new fixed point in I, we do not expect to find such drastically different behavior in the present case.

III. RENORMALIZATION-GROUP RECURSION FORMULAS

First we examine the Gaussian limit $u_0 = v_0 = 0$. The modified two-spin correlation function, defined in Eqs. (4) and (5), becomes, in this limit, the matrix inverse to $U_2^{\alpha\beta}(\vec{q})$, namely,

$$G^{\alpha\beta}(\vec{q}) = \frac{1}{\tau_0 + q^2 - f_0(q^\alpha)^2} \left(\delta_{\alpha\beta} - \frac{h_0 q^\alpha q^\beta}{[1 + h_0 \sum_\gamma (q^\gamma)^2 / [\tau_0 + q^2 - f_0(q^\gamma)^2]] [\tau_0 + q^2 - f_0(q^\beta)^2]} \right). \quad (24)$$

Thus, for any finite value of τ_0 , the limit of $G^{\alpha\beta}(\vec{q})$ for $\vec{q} \rightarrow 0$ is $1/\tau_0$, and we do not have the angular dependent terms that arose in I for the ferromagnetic case. However, for $\tau_0 = 0$ ($T = T_0$), or for $\tau_0 \ll q^2$, Eq. (24) becomes dependent on nonanalytic ratios such as $q^\alpha q^\beta / q^2$, with coefficients of order h_0 or f_0 . By our assumption (19), h_0 and f_0 are small compared to unity. Expanding (24) in powers of h_0 and f_0 for $\tau_0 = 0$ gives

$$G^{\alpha\beta}(\vec{q})|_{\tau_0=0} = \frac{1}{q^2} \left[\delta_{\alpha\beta} - h_0 \frac{q^\alpha q^\beta}{q^2} + f_0 \left(\frac{q^\alpha}{q} \right)^2 \delta_{\alpha\beta} + O(h_0^2, f_0^2, h_0 f_0) \right]. \quad (25)$$

Thus, the propagator $G^{\alpha\beta}$ has an angular dependence, which suppresses part of the longitudinal fluctuations (of order h_0). Propagator (24) would reduce to the pure "transverse" dipolar propagator discussed in I only for $h_0 \gg 1$ and $f_0 = 0$. This represents an isotropic or "liquid antiferromagnet," with a very strong dipolar interaction [contrary to assumption (19)]. We shall consider this case separately in Sec. IV. In the meanwhile, we restrict our discussion to small values of h_0 and f_0 , and use propagator (25), or the expansion of (24) in powers of h_0 and f_0 (for $\tau_0 \neq 0$). As we shall see, the only fixed-point value of h will turn out to be zero, so that this is the only interesting range of values of h_0 .

We can now proceed with the Feynman-graph expansion of $e^{\bar{\mathcal{H}}}$ in powers of u_0 and v_0 . The propagator $G^{\alpha\beta}(\vec{q})$ of (24) is used, with the previous renormalization procedure: integrating over $b^{-1} < |\vec{q}| < 1$, rescaling the spins by ξ_l , and expressing $\bar{\mathcal{H}}_{l+1}$ in terms of $\bar{\mathcal{H}}_l$. The details were given in Paper I, and yield

$$\begin{aligned} U_2^{l+1,\alpha\beta}(\vec{q}) = & \xi_l^2 b^{-d} \left[r_l + b^{-2} q^2 - b^{-2} f_l (q^\alpha)^2 \right] \delta_{\alpha\beta} + b^{-2} h_l q^\alpha q^\beta + 4 \left(\delta_{\alpha\beta} \sum_\gamma (u_l + v_l \delta_{\alpha\gamma}) \int_{\vec{q}_1} G^{\gamma\gamma}(\vec{q}_1) + 2 \int_{\vec{q}_1} G^{\alpha\beta}(\vec{q}_1) \right. \\ & - 32 \sum_{\gamma\delta} (u_l + v_l \delta_{\alpha\gamma})(u_l + v_l \delta_{\gamma\beta}) \int_{\vec{q}_1} \int_{\vec{q}_2} [G^{\alpha\beta}(\vec{q}_1) G^{\gamma\delta}(\vec{q}_2) G^{\gamma\delta}(\vec{q}_1 + \vec{q}_2 + b^{-1} \vec{q}) \\ & \left. + 2 G^{\alpha\gamma}(\vec{q}_1) G^{\delta\gamma}(\vec{q}_2) G^{\beta\delta}(\vec{q}_1 + \vec{q}_2 + b^{-1} \vec{q}) \right] + O(u_l^3, v_l^3, u_l^2 v_l, \dots) \quad (26) \end{aligned}$$

As before, $\int_{\vec{q}}$ denotes integration over the range $b^{-1} < |\vec{q}| < 1$. Comparison with (21) gives the recursion relation

$$\begin{aligned} r_{l+1} = & \xi_l^2 b^{-d} \{ r_l + 4K_d [(d+2)u_l + 3v_l] \\ & \times A^d(r_l, h_l, f_l) + O(u_l^2, v_l^2, u_l v_l) \}, \quad (27) \end{aligned}$$

where the basic integral A^d is

$$A^d(r, h, f) = \int_{b^{-1}}^1 \frac{q^{d-1} dq}{r + q^2} \left(1 + \frac{(f-h)q^2}{d(r+q^2)} + O(f^2, h^2, fh) \right), \quad (28)$$

and where $K_d^{-1} = 2^{d-1} \pi^{d/2} \Gamma(\frac{1}{2}d)$.

The $u_i^2, v_i^2, u_i v_i$ terms in (26) will contribute to the coefficients of $q^2, (q^\alpha)^2$, and $q^\alpha q^\beta$ in $U_2^{i+1, \alpha\beta}$. By repeating the arguments of I, we see that we need to calculate these terms only for $d=4, \gamma=0$. Thus, the relevant propagator is (25): This is precisely the propagator used in I, except for the factor h_i which multiplies $q^\alpha q^\beta / q^2$. Basically, the calculations of I also apply here. However, the situation is now somewhat simpler, since all the "angular" terms in propagator (25) are of order h or f . This enables us to carry these calculations a little further. Since, by assumption, h_0 and f_0 are small, we may also assume this for all l , derive the recursion formulas to first order in h_i

and f_i , and check the consistency of the results. The integrals entering the last term in (26) are of the form

$$X^{\alpha\beta\gamma\delta} = \int_{\vec{q}_1}^> \int_{\vec{q}_2}^> G^{\alpha\gamma}(\vec{q}_1) G^{\gamma\delta}(\vec{q}_2) \times [G^{\delta\beta}(\vec{q}_1 + \vec{q}_2 + b^{-1}\vec{q}) - G^{\delta\beta}(\vec{q}_1 + \vec{q}_2)] = \int_{\vec{q}_1}^> G^{\alpha\gamma}(\vec{q}_1) [I^{\gamma\delta\beta}(\vec{q}_1 + b^{-1}\vec{q}) - I^{\gamma\delta\beta}(\vec{q}_1)], \quad (29)$$

where we have subtracted the $\vec{q}=0$ contributions [which give the u_i^2, v_i^2 , and $u_i v_i$ terms in (27)]. To first order in h, f the integral $I^{\gamma\delta\beta}$ is

$$I^{\gamma\delta\beta}(\vec{q}) = \int_{\vec{q}_2}^> G^{\gamma\delta}(\vec{q}_2) G^{\delta\beta}(\vec{q}_2 + \vec{q}) = \delta_{\gamma\delta} \delta_{\delta\beta} \int_{\vec{q}_2}^> \frac{1}{q_2^2(\vec{q}_2 + \vec{q})^2} - h\delta_{\delta\beta} \int_{\vec{q}_2}^> \frac{q_2^\gamma q_2^\delta}{q_2^4(\vec{q}_2 + \vec{q})^2} - h\delta_{\gamma\delta} \int_{\vec{q}_2}^> \frac{(q_2^\beta + q^\beta)(q_2^\delta + q^\delta)}{q_2^2(\vec{q}_2 + \vec{q})^4} + f\delta_{\gamma\delta} \delta_{\delta\beta} \int_{\vec{q}_2}^> \frac{(q_2^\gamma)^2}{q_2^4(\vec{q}_2 + \vec{q})^2} + f\delta_{\gamma\delta} \delta_{\delta\beta} \int_{\vec{q}_2}^> \frac{(q_2^\beta + q^\beta)^2}{q_2^2(\vec{q}_2 + \vec{q})^4}. \quad (30)$$

Finally, we expect $X^{\alpha\beta\gamma\delta}$ to yield terms of the form $q^2 \ln b / b^2, q^\alpha q^\beta \ln b / b^2$, etc., since these will lead to recursion relations of the form

$$h_{i+1} = b^{-\eta_i^h} h_i,$$

with

$$\eta_i^h = O(u_i^2, u_i v_i, v_i^2),$$

and so on. For this purpose, it is convenient to assume $b \gg 1$, so that b^{-2} is negligible compared to $b^{-2} \ln b$.⁷ The factor $G^{\alpha\gamma}(\vec{q}_1)$ in (29) is at most of order $q_1^{-2} < b^2$. Hence logarithmic terms such as $\ln b$ can arise only from the factor $I^{\gamma\delta\beta}(\vec{q}_1 + b^{-1}\vec{q}) - I^{\gamma\delta\beta}(\vec{q}_1)$. Going back to (26), one can see that we actually need only combinations of the $I^{\gamma\delta\beta}$, such as $\sum_\delta I^{\gamma\delta\beta}, I^{\gamma\delta\beta}$, or $\sum_{\gamma\delta} I^{\gamma\delta\beta}$. Clearly, each of these combinations has at most two indices, γ and β , and hence may be represented as a linear combination of $\delta_{\gamma\beta}$ and of $q^\gamma q^\beta / q^2$, with coefficients which may depend on q^2 . For example, we have

$$J^{\gamma\delta}(\vec{q}) = \sum_\beta I^{\gamma\delta\beta}(\vec{q}) = a(q^2) \delta_{\gamma\beta} + b(q^2) q^\gamma q^\beta / q^2. \quad (31)$$

On writing $J^{\gamma\delta}(\vec{q})$ explicitly, it is easy to see that

$$da + b = \sum_\gamma J^{\gamma\gamma}(\vec{q}), \quad a + b = J^{11}(\vec{q}). \quad (32)$$

In the second equation of (32) we may choose \vec{q} parallel to the first axis, thus obtaining a simple integration. All one needs now, to find the coefficients a and b explicitly, are the formulas

$$\frac{2}{\pi} \int_0^\pi \frac{\sin^2 \theta d\theta}{q_1^2 + q_2^2 + 2q_1 q_2 \cos \theta} = \min\left(\frac{1}{q_1^2}, \frac{1}{q_2^2}\right) \quad (33)$$

and

$$\frac{2}{\pi} \int_0^\pi \frac{\sin^2 \theta d\theta}{(q_1^2 + q_2^2 + 2q_1 q_2 \cos \theta)^2} = \frac{1}{|q_2^2 - q_1^2|} \min\left(\frac{1}{q_1^2}, \frac{1}{q_2^2}\right). \quad (34)$$

Next we may form the difference $J^{\gamma\delta}(\vec{q}_1 + b^{-1}\vec{q}) - J^{\gamma\delta}(\vec{q}_1)$, and expand to order q^2 . This reveals that to obtain the factor $\ln b$ in the final integration over \vec{q}_1 , only the $\ln q$ term in $a(q^2)$ and the order unity term in $b(q^2)$ need be retained. The appropriate expression is thus

$$J^{\gamma\delta}(\vec{q}) \approx -\frac{1}{4} K_4 \delta_{\gamma\beta} (4 - 2h + 2f) \ln q - \frac{1}{2} h K_4 q^\gamma q^\beta / q^2 + \frac{1}{2} f K_4 (q^\gamma)^\beta / q^2 \delta_{\gamma\beta}. \quad (35)$$

Substituting this and similar results in (26) finally yields a contribution to $U_2^{i+1, \alpha\beta}(\vec{q})$ given by

$$\Delta U_2^{i+1, \alpha\beta}(\vec{q}) = -8K_4^2 b^{-2} \ln b \{ -\delta_{\alpha\beta} q^2 \times [6u_i^2 + 6u_i v_i + 3v_i^2 + O(u_i^2 h_i, u_i v_i h_i, v_i^2 h_i)] - \frac{1}{9} h_i q^\alpha q^\beta [30u_i^2 + 28u_i v_i] + \frac{1}{9} \delta_{\alpha\beta} (q^\alpha)^2 [30f_i u_i^2 + (48h_i - 32f_i) u_i v_i + 27(f_i - h_i) v_i^2] \} + O(u_i^2 h_i^2, u_i^2 h_i f_i, \dots). \quad (36)$$

The renormalized coefficient of q^2 is to be equat-

ed to unity by choice of the rescaling factor ζ_i . If we neglect the f_i and h_i contributions the result is

$$1 = \zeta_i^2 b^{-d-2} [1 + 24K_4^2(2u_i^2 + 2u_i v_i + v_i^2) \ln b], \quad (37)$$

which yields

$$\zeta_i^2 = b^{d+2-\eta_i}, \quad (38)$$

with exponent

$$\eta_i = 24K_4^2(2u_i^2 + 2u_i v_i + v_i^2). \quad (39)$$

The renormalized coefficients of $q^\alpha q^\beta$ and of $(q^\alpha)^\beta \delta_{\alpha\beta}$ then become

$$\begin{aligned} h_{i+1} &= b^{-\eta_i} [1 + K_4^2(\frac{80}{3}u_i^2 + \frac{224}{9}u_i v_i) \ln b] h_i \\ &= b^{-\eta_i^h} h_i, \end{aligned} \quad (40)$$

with

$$\eta_i^h = K_4^2(\frac{64}{3}u_i^2 + \frac{208}{9}u_i v_i + 24v_i^2) \quad (41)$$

and

$$\begin{aligned} f_{i+1} &= b^{-\eta_i} \{ [1 + K_4^2(\frac{80}{3}u_i^2 - \frac{256}{9}u_i v_i + 24v_i^2) \ln b] f_i \\ &\quad + K_4^2(\frac{128}{3}u_i v_i - 24v_i^2) \ln b h_i \} \\ &= b^{-\eta_i^f} f_i + b^{-\eta_i} K_4^2(\frac{128}{3}u_i v_i - 24v_i^2) \ln b h_i, \end{aligned} \quad (42)$$

where

$$\eta_i^f = K_4^2(\frac{64}{3}u_i^2 + \frac{688}{9}u_i v_i). \quad (43)$$

Thus, if v_i is small compared to u_i , both η_i^h and η_i^f are positive, and so both f_i and h_i decrease with increasing l . Thus, the initial assumption $h, f \ll 1$ is justified. Moreover, if $h_0, f_0 \ll 1$, the terms of order $u_i^2 h_i^2$, etc., in (36) are not capable of canceling the terms considered. Thus, unless v_i becomes large and negative (so that η_i^f becomes negative), h_i and f_i will go to zero as l goes to infinity. We have hence established that f and h are in irrelevant variables near any fixed point with $v=0$ and $g=0$ (such as the standard Heisenberg fixed point discussed in I). This increases the plausibility of our claim, in I, that the same probably holds also when $g \rightarrow \infty$.

To obtain recursion formulas for u_i and for v_i , we now turn to the Feynman graph (b) in Fig. 1, and follow the discussion that led to the relations (95) and (96) of I. Again, all the propagators are expanded to first order in h and in f . The final result is

$$\begin{aligned} u_{i+1} &= b^\epsilon \{ u_i - 4K_4 \ln b [(12 + 6h_i)u_i^2 \\ &\quad + (6 + 3h_i)u_i v_i] + 4K_4 \ln b \\ &\quad \times f_i [\frac{37}{10}u_i^2 + 3u_i v_i] + O(u_i^3, u_i^2 h_i^2, u_i^2 f_i^2, \dots) \} \end{aligned} \quad (44)$$

and

$$\begin{aligned} v_{i+1} &= b^\epsilon \{ v_i - 4K_4 \ln b [(12 + 5h_i)u_i v_i \\ &\quad + (9 + \frac{9}{2}h_i)v_i^2] + 4K_4 \ln b \end{aligned}$$

$$\times f_i [6u_i v_i + \frac{9}{2}v_i^2] + O(v_i^3, v_i^2 f_i^2, \dots) \}, \quad (45)$$

where the $\ln b$ factor arises from an integration of a product of two propagators with $r=h=f=0$.

IV. FIXED POINTS AND CRITICAL BEHAVIOR

Clearly, for $v=f=h=0$ the recursion relations for r and for u reduce simply to those for the normal d -component Heisenberg antiferromagnet.^{8,9} Indeed, from Eqs. (40), (42), and (45) we see that $v^*=f^*=h^*=0$ are solutions, which yield the Heisenberg fixed point

$$v^*=f^*=h^*=0, \quad K_4 u^* = \frac{1}{48} \epsilon, \quad r^* = -\frac{1}{4} \epsilon. \quad (46)$$

Moreover, if $v=0$, this remains a stable fixed point, as discussed above. The other nontrivial fixed point, $u^*=0$ and $v^*=\frac{1}{36}\epsilon$, is unstable with respect to u , and leads back to (46).

The case $v \neq 0$ has to be given special attention. It has already been noted in I that v is also a relevant parameter in some cases. Actually, as found by Wegner,¹⁰ the "exponent" $\lambda_v = d - \omega_v = 1/\nu_v$ for v ($x_{0\epsilon}$ in Wegner's notation) is equal to $(n-4)\epsilon/(n+8) + O(\epsilon^2)$ near the Heisenberg fixed point. This vanishes to order ϵ for $n=d$, and it is necessary to calculate higher-order terms. In the Appendix we present a second-order calculation, which uses all the graphs of Fig. 1 and yields the full recursion relations for u and v near the Heisenberg fixed point. The result, for $n=4-\epsilon$, is $\lambda_v = \frac{1}{12}\epsilon^2$, so that the Heisenberg fixed point is actually unstable with respect to v . However, in first order in f and h , to which we are working, no v terms are produced during renormalization, since the coefficient of $f_i u_i^2$ in (45) vanishes identically! If v_i is generated, it must be from terms of order $f_i h_i u_i^2$. We can now repeat the arguments of Sec. VIII of I, and show that, since the crossover exponent for v is only $\phi_v = \frac{1}{24}\epsilon^2$, one will have to approach very close indeed to T_c in order to detect significant deviations from the Heisenberg critical exponents. These ex-

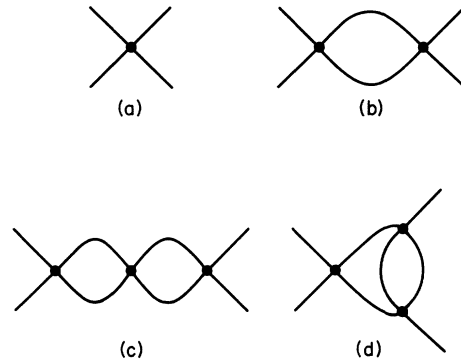


FIG. 1. Feynman graphs for the recursion relations for u and for v .

ponents may, of course, be found simply by using Wilson's results^{11,13} to order ϵ^2 , with $n = d = 4 - \epsilon$, which yield

$$2\nu = 1 + \frac{1}{4}\epsilon + \frac{1}{8}\epsilon^2 + O(\epsilon^3). \quad (47)$$

Combining (46) with (39) gives

$$\eta = \frac{1}{48}\epsilon^2 + O(\epsilon^3), \quad (48)$$

in agreement with Wilson's result from a Feynman-graph expansion.¹¹ Finally, Eqs. (41) and (43) now give

$$\eta^h = \eta^f = \frac{1}{108}\epsilon^2 + O(\epsilon^3). \quad (49)$$

We can now repeat the arguments of Sec. VII of I to derive the form of the correlation function. As in the usual case, the order ϵ terms in the expansion of $G_i^{\alpha\beta}(b^i\vec{q})$ cancel, and for $\xi q \ll 1$, we finally find

$$\begin{aligned} \Gamma^{\alpha\beta}(\vec{q}) &= b^{1(2-\eta)}\Gamma_i^{\alpha\beta}(\vec{q}b^i) \\ &\approx \frac{Ct^{-\nu}}{1 + \xi^2 q^2} \left(\delta_{\alpha\beta} - \frac{h_0 \xi^{2-\eta^h} q^\alpha q^\beta}{1 + \xi^2 q^2} \right. \\ &\quad \left. + \delta_{\alpha\beta} \frac{f_0 \xi^{2-\eta^f} (q^\alpha)^2}{1 + \xi^2 q^2} + O(\epsilon^2, h_0^2, f_0^2) \right), \end{aligned} \quad (50)$$

where

$$t = (T/T_c) - 1, \quad (51)$$

$$\xi \approx \xi_0 t^{-\nu}, \quad (52)$$

$$\nu = (2 - \eta)\nu = 1 + \frac{1}{4}\epsilon + \frac{11}{96}\epsilon^2 + O(\epsilon^3). \quad (53)$$

We may note that the η^h and η^f contributing to the expression (50) are of order ϵ^2 , and so may actually be included in the last term. Only for $h_0(q\xi)^2$, $f_0(q\xi)^2 \ll 1$ will the corrections to the usual Heisenberg behavior be negligible.

Since f and h are irrelevant parameters, their limits as $T \rightarrow T_c$ are zero, hence the asymptotic correlation function at the critical point (ignoring a possible generation of ν terms) will be unaffected by these corrections, and we shall have^{8,11}

$$\Gamma_c^{\alpha\beta}(\vec{q}) \approx C'/q^{2-\eta} \quad (q \rightarrow 0), \quad (54)$$

with η given by (48). However, it must be emphasized that the approach of (50) to (54) is very slow, and thus less-singular higher-order terms of order

$$h(q^\alpha q^\beta / q^2) / q^{2-\eta-\eta^h}$$

and

$$f\delta_{\alpha\beta}(q^\alpha/q)^2 / q^{2-\eta-\eta^f}$$

in (54), may play an important role in practice.

The staggered susceptibility is related to $\Gamma^{\alpha\beta}(0)$, and hence is not affected by any of the corrections to (50), since

$$\chi \propto \Gamma^{\alpha\alpha}(0) = Ct^{-\nu}. \quad (55)$$

It may be worth stressing, that shape-dependent

effects are absent only from the staggered susceptibility, but can appear in the real susceptibility, given, in our notation, by $\Gamma^{\alpha\beta}(-\vec{k}_0)$ (see also Sec. VII of I).

If f_0 and h_0 are not very small, then higher-order terms may eventually generate ν terms, which will lead away from the Heisenberg fixed point. To estimate this one has to go beyond the linear approximation in h and in f .

The domain of large f values is rather hard to handle, owing to the complicated form of the full propagator (24). However, if f is small, the domain of large h can be treated quite generally. In particular, on assuming $f=0$ (a "liquid antiferromagnet"), the expression (25) becomes

$$G^{\alpha\beta}(\vec{q})|_{r_0=0} = \frac{1}{q^2} \left(\delta_{\alpha\beta} - y \frac{q^\alpha q^\beta}{q^2} \right), \quad (56)$$

with

$$y = h_0/(1 + h_0). \quad (57)$$

We can now repeat all the calculations of Sec. III, finally finding that the recursion relation (40), with $\nu_i = 0$, becomes

$$h_{i+1} = b^{-\eta_i} [h_i + 32K_4^2 u_i^2 (\frac{5}{8}y_i - \frac{1}{8}y_i^2 + \frac{1}{8}y_i^3)]. \quad (58)$$

At the same time, relation (39) is replaced by

$$\eta_i = 32K_4^2 u_i^2 (\frac{3}{2} - \frac{4}{3}y_i + \frac{19}{24}y_i^2 - \frac{1}{8}y_i^3). \quad (59)$$

Substituting (59) in (58) and solving for h^* immediately shows that $h^* = 0$ is the only real fixed point of (58). (There are two other imaginary solutions.) Hence, for small values of f and of ν the Heisenberg fixed point describes the critical behavior, even for a large isotropic dipolar interaction! A general treatment for nonzero f and ν is, of course, still wanted.

It is interesting to note, that when $y=1$ the propagator (56) reduces to the form discussed in I for a ferromagnet near the dipolar fixed point. Putting $y=1$ in (59) yields $\eta_{\text{dip}} = \frac{80}{3}K_4^2 u^{*2}$, in agreement with the Feynman-graph expansion result derived in Paper II.²

V. DISCUSSION

We now consider briefly the other cubic lattices, namely, the bcc and fcc lattices. It is difficult to proceed with explicit forms, such as (9), for both cases. For the bcc lattice, if we choose the lattice points as $(a/3^{1/2})(n_1, n_2, \dots)$ and let the even n_i determine one sublattice and the odd ones the other, then the shortest distance between two points on different sublattices is $a(\frac{1}{3}d)^{1/2}$, whereas the shortest distance between two points in the same sublattice is $2a/3^{1/2}$. Thus, for d near 4 the assumption made in deriving (9) is unjustified. The fcc case is even more tricky, since even in three dimensions there

are no simple antiferromagnets with only nearest-neighbor exchange interactions.

To generalize, therefore, it is appropriate to allow more than nearest-neighbor interactions, and to study the full Fourier transform $\hat{J}(\vec{k})$ as in (7). If this function has an absolute maximum at some point \vec{k}_1 in \vec{q} space, which indicates a possible type of ordering, we can expand \hat{J} about \vec{k}_1 , as in (9), and then proceed as in the text. In this case, identity (10) may fail, which could amount to a shift in the mean field critical temperature T_0 of (22). Otherwise all the expressions remain unchanged, and the results are hence applicable to any cubic antiferromagnet.

We thus conclude that the critical behavior of ferromagnets and antiferromagnets very close to T_c is generally different: the former are strongly affected by the dipolar forces, while the latter experience only slight changes due to these interactions. This shows that arguments of "universality" must be used with due caution! The differences between otherwise comparable antiferromagnets and ferromagnets have, in fact, been indicated in experiments⁴ on RbMnF_3 and EuO , as discussed in Ref. 3. The specific-heat exponents for these materials may be estimated as -0.14 ± 0.05 and -0.04 ± 0.03 , respectively.^{3,4} Indeed, the Heisenberg value of the specific-heat exponent is⁸⁻¹⁰

$$a \approx \frac{4-d}{2(d+8)} \epsilon - \frac{(d+2)^2(d+28)}{4(d+8)^2} \epsilon^2 = -\frac{1}{8} \epsilon^2, \quad (60)$$

whereas the dipolar exponent, found in I, is

$$\alpha = -\frac{1}{34} \epsilon + O(\epsilon^2). \quad (61)$$

For $\epsilon = 1$, these truncated expressions yield -0.13 and -0.03 , respectively! Of course, these values are based on the unjustified neglect of the unknown $O(\epsilon^2)$ terms in the dipolar case, which might well be large as in (60). However, even though the concordance with the experimental results is probably coincidental, it is quite suggestive.

More generally, our results indicate that for antiferromagnets with relatively large dipolar interactions, measurements of the correlation functions and thermodynamic properties may reveal complicated (i. e., crossover) behavior over quite a wide range of temperatures near T_c .

Another problem to which the present theory may be applied rather directly concerns anisotropic ferromagnets, in which the anisotropy has the angular dependence of (1), except for a replacement of $|\vec{R} - \vec{R}'|^{-d}$ by a short-range function. As pointed out by Van Vleck,¹² this may represent the spin-orbit parts of the exchange integral. When one goes through the calculation of the Fourier transform (8), one now discovers that the term $q^\alpha q^\beta / q^2$ does

not appear [as noted in I, this term is related to the long-range character and to the shape dependence of $A^{\alpha\beta}(0)$, which does not exist for a short-range potential]. Thus, the expansion of $A^{\alpha\beta}(\vec{k})$, now about $\vec{k} = 0$, will have a form similar to (11) (with $\vec{k}_0 = 0$). We conclude that the Heisenberg fixed point is also appropriate for the description of such a system, unless the parameter f_0 [or b_5 in Eq. (11)] becomes large. Clearly, this strongly anisotropic case still needs further investigation.

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APPENDIX: INSTABILITY OF THE RECURSION RELATION FOR ν NEAR THE HEISENBERG FIXED POINT

In the linear region near the Heisenberg fixed point, the propagator is simply

$$G^{\alpha\beta}(\vec{q}) = \delta_{\alpha\beta} / (r + q^2). \quad (A1)$$

To third order in u and in v , we have to consider the Feynman graphs shown in Fig. 1. For graphs (c) and (d) of Fig. 1 we may perform the appropriate integrals with $r = 0$ and $d = 4$, thus finding

$$\int_{\vec{q}_1}^{\vec{q}_2} \int_{\vec{q}_2}^{\vec{q}_1} G^{\alpha\beta}(\vec{q}_1) G^{\gamma\delta}(\vec{q}_1) G^{\epsilon\eta}(\vec{q}_2) G^{\xi\chi}(\vec{q}_2) \\ = \delta_{\alpha\beta} \delta_{\gamma\delta} \delta_{\epsilon\eta} \delta_{\xi\chi} K_4^2 \ln^2 b \quad (A2)$$

for graph (c), and

$$\int_{\vec{q}_1}^{\vec{q}_2} \int_{\vec{q}_2}^{\vec{q}_1} G^{\alpha\beta}(\vec{q}_1) G^{\gamma\delta}(\vec{q}_1) G^{\epsilon\eta}(\vec{q}_2) G^{\xi\chi}(\vec{q}_1 + \vec{q}_2) \\ = \delta_{\alpha\beta} \delta_{\gamma\delta} \delta_{\epsilon\eta} \delta_{\xi\chi} K_4^2 \left[\frac{1}{2} \ln b + \frac{1}{2} \ln^2 b + O(b^{-2}) \right] \quad (A3)$$

for graph (d). We shall be interested only in the logarithmic terms, assuming $b \gg 1$, since we finally want to find the appropriate exponents.⁷ For graph (b) we need to keep terms of order ϵ , which leads to

$$\int_{\vec{q}}^{\vec{q}} G^{\alpha\beta}(\vec{q}) G^{\gamma\delta}(\vec{q}) = K_d \left[\ln b + \frac{1}{2} \epsilon \ln^2 b + O(\epsilon b^{-2}) \right] \delta_{\alpha\beta} \delta_{\gamma\delta}. \quad (A4)$$

For each vertex we have to multiply by $-(u + \delta_{\alpha\beta} v)$, where α and β are the indices of the two pairs of lines entering the vertex. Finally, we find—for n -component spins—

$$u' = b^{\epsilon-2\eta} \left\{ u - 4K_d \ln b \left(1 + \frac{1}{2} \epsilon \ln b \right) [(n+8)u^2 + 6uv] + 16K_d^2 \ln^2 b [u^3(n^2 + 6n + 20) + u^2v(9n + 36) + 27uv^2] \right. \\ \left. + 32K_d^2 \ln b (1 + \ln b) [u^3(5n + 22) + 36u^2v + 9uv^2] \right\} + \dots, \quad (\text{A5})$$

$$v' = b^{\epsilon-2\eta} \left\{ v - 4K_d \ln b \left(1 + \frac{1}{2} \epsilon \ln b \right) (12uv + 9v^2) + 16K_d^2 \ln^2 b (36u^2v + 54uv^2 + 27v^3) \right. \\ \left. + 32K_d^2 \ln b (1 + \ln b) [(3n + 42)u^2v + 72uv^2 + 27v^3] \right\} + \dots. \quad (\text{A6})$$

The η in the exponent of the coefficients of these equations follows the spin-normalization relation

$$\zeta^2 = b^{d+2-\eta}. \quad (\text{A7})$$

Thus, $v^* = 0$ is a fixed point value. Assuming $u^* \neq 0$, we find

$$K_d u^* = \frac{\epsilon}{4(n+8)} \left(1 + \frac{9n+42}{(n+8)^2} \epsilon + O(\epsilon^2) \right), \quad (\text{A8})$$

where we have used

$$\eta = [(n+2)/2(n+8)^2] \epsilon^2. \quad (\text{A9})$$

We can now linearize the recursion relations near $v^* = 0$ and u^* , as given by (A8), and find the eigenvalues. The result for the eigenvalue of v is

$$b^{\lambda_v} = 1 + \epsilon \ln b \frac{n-4}{n+8} - 2\eta \ln b \\ + \epsilon^2 \ln b \frac{6(n^2+4n+28)}{(n+8)^3} + \frac{1}{2} \epsilon^2 \ln^2 b \left(\frac{n-4}{n+8} \right)^2, \quad (\text{A10})$$

whereas the eigenvalue of u is $b^{-\epsilon} + O(\epsilon^2)$, as usual. Clearly, λ_v is of order ϵ^2 for $n=4$. Letting $n=d=4-\epsilon$, we find

$$\lambda_v = \frac{1}{12} \epsilon^2 + O(\epsilon^3). \quad (\text{A11})$$

It may be noted that for any $n \geq 4$, v is a relevant variable, which may affect critical exponents. (This even includes the spherical model limit!)

If $v_0 = 0$, and the equation for v is (A6), no v will be generated by the renormalization procedure, and the positive exponent of v gives no cause for concern. However, any perturbation which reduces the rotational symmetry to the cubic symmetry [e.g., f_0 in Eq. (21)] may lead to a nonzero v . This then results either in a new fixed point, with new exponents, or in a first-order phase transition (as

is the case for the Baxter-like model discussed by Wilson and Fisher¹³).

It may be noted that result (A8) for u^* can now be used in the recursion relation for r , to yield the exponent ν to second order in ϵ . The results are in agreement with those obtained by Wilson's Feynman-graph expansion to second order.¹¹ It is also appropriate to note that we have ignored altogether the irrelevant variables, since their contribution to order ϵ^2 does not involve $\ln b$, and therefore they do not affect the critical exponents.

It is interesting to note that even for $n=3$ and $\epsilon=1$, $\lambda_v = 0.0887 > 0$, and hence v is a relevant variable! For $n=2$ the order ϵ^2 term exactly cancels the order ϵ term, and so $\lambda_v = O(\epsilon^3)$. This answers Wegner's¹⁰ question concerning the perturbation Og , proving that indeed this perturbation is important and may affect critical exponents for $n > 2$, although, as was shown, its related cross-over exponent is small and hence the effects are expected to be felt only very close to T_c . This problem is further investigated in Ref. 15.

An interesting by-product of the present calculation is the eigenvalue of the equation for u , which is

$$\lambda_u = -\epsilon + [(9n+42)/(n+8)^2] \epsilon^2 + O(\epsilon^3). \quad (\text{A12})$$

This is equal to Wegner's¹⁰ $d - x_{2s}$. It is clear from (A12), that the order ϵ^2 terms are very important, as they change λ_u by nearly a factor of 2. The exponent Δ_u for the leading correction¹⁴ to the scaling laws now becomes

$$\Delta_u = -\nu \cdot \lambda_u = \frac{1}{2} \epsilon - \frac{68+8n-n^2}{4(n+8)^2} \epsilon^2, \quad (\text{A13})$$

which gives $\Delta_u = 0.269$ for $n=1$ and $\Delta_u = 0.329$ for $n=3$, and thus makes this correction quite important!

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$\exp(i\vec{k}_0 \cdot \vec{R}_l) = -1$. For a sphere around the origin, each of these sums will vanish by cubic symmetry. For a large enough sphere, we can accurately approximate the two sums outside the sphere by integrals, which will have equal numerical values. Since they have opposite signs, their contributions will precisely cancel.

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These authors do not actually calculate the coefficients b_4 , b_5 , and b_7 , but the values may be estimated by taking finite difference in their tables of $A^{ab}(\vec{q})$.

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