Some developments in the theory of modulated order. I. The role of fluctuations in the axial next-nearest-neighbor Ising model and the relevance of the Thouless-Anderson-Palmer equation

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The general mean-field theory of systems with modulated order is extended so as to include nontrivial fluctuation effects through the use of the Kirkwood approximation. Application of the theory to the axial next-nearest-neighbor Ising (ANNNI) model reveals that fluctuations (1) decrease the size of the entire ordered region of the phase diagram, (2) decrease that fraction of the ordered region that is most highly modulated, and (3) suppress the reentrant parts of the modulated region that do survive. Physical reasons for this behavior are discussed. In addition, we note that our ANNNI mean-field equations turn out to be precisely the Thouless-Anderson-Palmer (TAP) equations of spin-glass theory despite a number of rather different assumptions made in deriving the TAP equations. Some of what this observation reveals about the TAP equations is discussed.

I. INTRODUCTION

From a historical perspective, the study of modulated order in solids is at a stage comparable to the earliest days of the study of ferromagnetic order with the Ising model. The simplest mean-field theory has been worked out for the simplest spin model showing interesting effects, namely the axial next-nearest-neighbor Ising (ANNNI) model.[1-3] However, the effects of going beyond mean-field theory, so as to include fluctuations, and the effects of changing the models, have yet to be considered in any systematic way. The beginning of just such a study will be the goal of this and the succeeding paper.[4]

One could, of course, make the argument that little will be gained from this kind of study. For Ising-like systems it turned out that neither the inclusion of fluctuations nor small changes in the models made much of a difference in the global structure of the phase diagram. To be sure, application of renormalization-group methods led to a dramatic revision of our ideas about behavior near critical points, but the "topology" of the Ising phase diagram has remained unchanged from that predicted by the original Curie-Weiss—Bragg-Williams mean-field theory.[5]

Nonetheless, on experimental grounds alone, it is clear that richer possibilities of modulated order leave us with a wealth of questions unanswered at our current level of understanding. For example, the rare-earth alloy Er_xTb_{1-x} exhibits two different ground-state magnetic orderings depending on the value of x, but at higher temperatures a third kind of ordering is observed which does not correspond to an experimental ground-state pattern.[6] In other words, there are modulated, ordered phases which are not energetically stable (and are therefore not ground states) but which become stable under the influence of thermal fluctuations. Even assuming that such fluctuations will never stabilize any ordered phase in an absolute sense, we are left with the questions—which are unanswerable at the mean-field level—of just how and when fluctuations favor one modulated structure over another.

In posing these questions, one is not limited to examples involving magnetic systems. Modulated order at finite temperatures is ubiquitous, with instances ranging from the pseudo-one-dimensional ordering implicit in the formation of staged graphite intercalation compounds[7] to the two-dimensional ordering of surface superlattices[8] to the fully-three-dimensional patterns defined by crystal structures.[9] One has no reason to suppose fluctuations should even play the same role in these different dimensionalities much less be equally ignorable.

What we will do in this paper is to consider what fluctuations do in the best studied modulated-order model, the ANNNI model.[1-3,10] In models of this sort, Ising spins are assumed to interact ferromagnetically with all their nearest-neighbor spins, but along one specified direction there is also an antiferromagnetic next-nearest-neighbor interaction. The competition between the ferromagnetic and antiferromagnetic forces gives rise to at least the possibility of a variety of magnetization patterns along the unique axis of the system. Parenthetically, the extent to which this notion of competing forces is a necessary component of models exhibiting modulated order (and, for that matter, the extent to which it is the central feature of the ANNNI model itself) is a subject which will be deferred until the next paper.[4] For the remainder of this article we will assume the paradigm of competing forces, confining ourselves to the question of what happens to the different energetically favorable ground-state patterns once the temperature is raised above $T=0$.

From low-temperature expansions it is known that the ANNNI model has an infinite number of modulated phases in the vicinity of the $T=0$ multiphase point.[11] The remainder of the phase diagram has been studied extensively with mean-field theory, revealing a complex sequence of transitions between phases occurring as the temperature is increased—a sequence that may very well

be a devil's staircase.[12] Once the temperature gets high enough to be close to the paramagnetic boundary, the mean-field equations can then be solved analytically.[3] These linearized equations indicate the existence of patterns of all possible periodicities—including irrational, and therefore incommensurate, ones. Thus the ANNNI model also exhibits a commensurate-incommensurate transition.[13]

The mean-field equations themselves are an infinite set of coupled nonlinear equations for the average magnetization of each layer perpendicular to the unique axis. As with any problem with nonuniform ordering, there is no single-order parameter which solves these equations. Rather, the set of layer magnetizations can be thought of as an "order-parameter function," much as is necessary to the study of spin glasses.[14] Had we reason to expect pure sinusoidal patterns, the task of finding this order-parameter function would simply be one of determining a few Fourier components, but this is unfortunately not the case. In practice,[2] the hierarchy of mean-field equations must be closed into coupled sets of P equations by assuming structures with periodicity P. However, not only does this approach preclude looking for incommensurate phases (since P must be integral), but even the resulting finite set of equations requires a root search which is nonergodic in a way which is also reminiscent of spin glasses.[15,16] The character of the solution to the root search inevitably mimics the character of the starting guess, so one is clearly not sampling the space of possible magnetization with any degree of completeness.

By way of anticipating our results, we might note that these analogies with spin glasses should not be entirely unexpected. As with spin glasses, the ANNNI model has a mixture of ferromagnetic and antiferromagnetic interactions, leading to an infinite number of ground states. If one further considers the ratio of antiferromagnetic to ferromagnetic interaction strength to be analogous to the width of the coupling-constant distribution[4] in the spin glass, even the global phase diagrams are closely related: the paramagnetic, ferromagnetic, and nontrivially ordered phases occur in the same places in the two models.[17] Apparently there has to be some fundamental distinction, in that the ferromagnetic-antiferromagnetic competition in the spin glasses arises out of a quenched-in distribution of coupling constants.[18] However, as we shall show in the companion paper,[4] even this distinction is somewhat illusory. We will be able to show that the ANNNI model is actually isomorphic to a random Ising model with annealed (correlated) nearest-neighbor couplings and that the vague analogy between the ANNNI and spin-glass phase diagrams can be made a little more precise.

Our goal in this paper of course is not to seek such connections but simply to explore the effect of fluctuations in the ANNNI model. In the next section we will do so by quite literally, retracing part of the history of the Ising model which we alluded to in the first paragraph of this section. Although this history seems largely to have been swept away under the onslaught of renormalization-group techniques,[19] there was at one time considerable effort devoted to making systematic improvements in mean-field theories. Because the improvements still led to classical exponents for critical phenomena, the approaches associated with the names of Kirkwood,[20] Bethe,[21] and Kikuchi[22] (for example) were quite naturally displaced as theories of critical phenomena. Still, with the advent of the richer phase diagrams afforded by models of modulated order, it is perhaps not inappropriate to use these methods to ask again the same question which has already been answered for the Ising model: how will our phase diagram be affected by fluctuations? A preliminary step in this direction was recently taken by Taylor and Desjardins,[23] who studied the ANNNI model in the Bethe approximation.[24] We will use the closely related Kirkwood approximation to the same end but, intriguingly, it will turn out that our particular choice leads precisely to the TAP equation, the same equation Thouless, Anderson, and Palmer used to study spin glasses.[25,26]

II. APPLICATION OF THE KIRKWOOD APPROXIMATION

The approximation that Kirkwood[20] developed in 1938 for the Ising model was one of the very first applications of what has become a standard approach to many-body systems: expansion of the free energy for the full interacting system, F, about that of some noninteracting reference system, F_0, as a series of cumulants in the interaction energy.[27] Quite generally, if one writes the full Hamiltonian as

$$\mathscr{H}=\mathscr{H}_0+V\,, \tag{2.1}$$

where $\mathscr{H}_0$ is the reference Hamiltonian and V is the interaction term, then the exact partition function Q can be written in terms of the reference partition function Q_0 and an average in the reference system,

$$\begin{aligned} Q&=\mathrm{Tr}e^{-\beta(\mathscr{H}_0+V)}\\ &=\mathrm{Tr}e^{-\beta\mathscr{H}_0}[\mathrm{Tr}(e^{-\beta\mathscr{H}_0}e^{-\beta V})/\mathrm{Tr}e^{-\beta\mathscr{H}_0}]\,,\\ Q&=Q_0\langle e^{-\beta V}\rangle_0\,, \end{aligned}$$

which sets up the free energy perfectly to be expanded in cumulants. Defining the relevant cumulants

$$\begin{aligned} \ln\langle e^{-\beta V}\rangle_0&=\ln\left[\sum_{n=0}^{\infty}(1/n!)(-\beta)^n\langle V^n\rangle_0\right]\\ &=\sum_{n=1}^{\infty}(1/n!)(-\beta)^nC_n(V) \end{aligned} \tag{2.2}$$

quickly enables us to write the free energy as desired,

$$-\beta F=\ln Q=-\beta F_0+\sum_{n=1}^{\infty}(1/n!)(-\beta)^nC_n(V) \tag{2.3}$$

In practice, the phrase "mean-field theory" usually means to take this expansion and truncate it at the $n=1$ level. However, with the exception of the first cumulant, which is simply the average interaction energy,

$$C_1(V)=\langle V\rangle_0\,, \tag{2.4a}$$

the cumulants represent the *fluctuations*

$$C_2(V)=\langle(V-\langle V\rangle_0)^2\rangle_0$$
$$=\langle V^2\rangle_0-\langle V\rangle_0^2\,,$$
$$C_3(V)=\langle(V-\langle V\rangle_0)^3\rangle_0\,, \tag{2.4b}$$
$$C_4(V)=\langle(V-\langle V\rangle_0)^4\rangle_0-3\langle(V-\langle V\rangle_0)^2\rangle_0^2\,,$$

so that one has to go to an order beyond $n=1$ to build any of the effects of fluctuations into the theory, besides those due to just the noninteracting reference. In this language, what Kirkwood did, essentially, was to truncate Eq. (2.3) at $n=2$. Though his procedure still led to a mean-field theory in the sense of giving classical critical exponents (as would truncating at any finite order),[28] the inclusion of nontrivial fluctuation corrections turned out to give a significant quantitative improvement over the Curie-Weiss theory.

Ideas of this sort have certainly been commonplace in the literature of solid-[29] and liquid-[30] state physics for many years. Indeed, for the vast majority of cases, the form of Eq. (2.3) that one would employ would be diagrammatic, with the possibility of one or more topological reductions (renormalizations) being performed before the calculation was started. The series might even be summed to infinite order in some approximate fashion. For our limited purpose of simply seeing the role of fluctuations, such an approach is less direct than the Kirkwood approximation. Before applying this approximation to a modulated-order problem in Sec. II B, however, we will first take the opportunity to review the analogous treatment of a uniformly ordered system. We do so not only for completeness and to cast Kirkwood's somewhat obscure derivation into a more modern language, but also to make a few technical points about the effect of system-wide constraints and the order-N^{-1} terms they give rise to. The importance of the same kind of terms in the non-uniformly-ordered theory will, we hope, be rendered somewhat less mysterious thereby.

A. A uniform system: The Ising ferromagnet

The ferromagnetic nearest-neighbor Ising model is the canonical example of a uniformly ordered system and is the case Kirkwood originally considered (in the model's binary-alloy incarnation). We will start by considering the more general Ising model described by the Hamiltonian

$$-\beta\mathcal{H}=\sum_{j,k}K(j,k)\mu_j\mu_k+\sum_j h(j)\mu_j\,, \tag{2.5}$$

where the μ's are Ising variables ($\mu=\pm1$), $K(j,k)+K(k,j)$ is the interaction between spins on sites j and k, and $h(j)$ is the magnetic field at site j (the interaction and the field both measured in units of $-kT$). Each sum runs over all N lattice sites. For much of the calculation, the interactions can be taken as arbitrary but short ranged, though we will adopt the conventions $K(j,k)=K(k,j)$ and $K(j,j)=0$. Thus the normal Ising ferromagnet corresponds to the choice

$$K(j,k)=\beta J/2 \quad j,k \text{ nearest neighbors}\,,$$
$$K(j,k)=0 \quad \text{otherwise}\,. \tag{2.6}$$

We define the order parameter for uniform ordering as the magnetization, given by

$$m=N^{-1}\sum_j\mu_j\,. \tag{2.7}$$

Note that Eq. (2.7) is a constraint which must be satisfied when evaluating sums over configurations. At the end of the calculation the value of m is determined so as to minimize the free energy, Eq. (2.3), but it is worth pointing out that Eq. (2.7) commits us to look for uniform order *regardless of the interactions*. Superficially, there seems to be a paradox here. We have a single-order parameter characteristic of a uniformly ordered state, yet the Hamiltonian, Eq. (2.5), includes the ANNNI model as a special case. In fact if we were to carry out this calculation for the ANNNI Hamiltonian, we would indeed find a solution (at least within a certain range of coupling-constant values) but we would have ignored the essential physics of the model by neglecting the possibility of modulated order. We will rectify this problem in Sec. II B, but the lesson is that equations such as (2.7) are hardly innocuous. We feel that some authors have been somewhat careless in this regard when discussing annealed random Ising models, but we defer discussion to the companion paper.[4]

Explicitly assuming uniform order then, the first step in our calculation is to break up the Hamiltonian as indicated in Eq. (2.1),

$$-\beta\mathcal{H}_0=\sum_j h(j)\mu_j\,,$$
$$-\beta V=\sum_{j,k}K(j,k)\mu_j\mu_k\,. \tag{2.8}$$

Both because it is needed for Eq. (2.3) and because of its applicability as a generating function for cumulants, we must next evaluate the free energy of the noninteracting system. However, due to the condition embodied by Eq. (2.7), there are still infinitely weak, infinitely long-range correlations present. An easy way to deal with this complication is to switch ensembles, which we do by introducing a Lagrange multiplier λ that will allow us to sum *independently* over all the spins in evaluating the noninteracting partition function,

$$Q_0(m)=\mathrm{Tr}\left\{e^{-\beta\mathcal{H}_0}\exp\left[-\lambda\left[Nm-\sum_j\mu_j\right]\right]\right\}. \tag{2.9}$$

The constraint will then be satisfied if λ is chosen so that

$$\frac{d\ln Q_0(m)}{d\lambda}=0\,. \tag{2.10}$$

On carrying out the trace indicated in Eq. (2.9), we arrive at the reference free energy

$$-\beta F_0(m)=\ln Q_0(m)$$
$$=-\lambda Nm+\sum_j\ln\{2\cosh[h(j)+\lambda]\}\,, \tag{2.11}$$

with λ determined from Eq. (2.10) as a solution of

$$\sum_j\tanh[h(j)+\lambda]=Nm\,. \tag{2.12}$$

In zero field, these equations can be combined to give

$$-\beta F_0/N = -[(1+m)/2]\ln[(1+m)/2] - [(1-m)/2]\ln[(1-m)/2] = -\int_0^m \tanh^{-1}x\,dx + \ln 2 , \quad (2.13)$$

the familiar Bragg-Williams result[5] for the entropy of a system of Ising spins at fixed magnetization m.

The entire Bragg-Williams theory results, as we have previously mentioned, from the $n=1$ truncation of Eq. (2.3). Were this our only goal, we would therefore need only one cumulant

$$-\beta C_1(V) = -\beta\langle V\rangle_0 = \sum_{j,k} K(j,k)\langle \mu_j\mu_k\rangle_0 , \quad (2.14)$$

which can be evaluated simply by considering Eq. (2.11) as a generating function. In particular, since it is straightforward to use Eq. (2.11) to calculate the multisite generalizations[27] of the cumulants of Eq. (2.4),

$$\begin{aligned} C(\mu_j) &= \langle \mu_j\rangle_0 = \partial(-\beta F_0)/\partial h(j) , \\ C(\mu_j\mu_k) &= \langle \mu_j\mu_k\rangle_0 - \langle \mu_j\rangle_0\langle \mu_k\rangle_0 \\ &= \partial^2(-\beta F_0)/\partial h(j)\partial h(k) , \\ C(\mu_j\mu_k\mu_l) &= \partial^3(-\beta F_0)/\partial h(j)\partial h(k)\partial h(l) , \\ C(\mu_j\mu_k\mu_l\mu_m) &= \partial^4(-\beta F_0)/\partial h(j)\partial h(k)\partial h(l)\partial h(m) , \end{aligned} \quad (2.15)$$

it is convenient to compute not only the moment we need here, but also the higher moments in terms of these cumulants (as shown in Table I). Thus, taking care to include the dependence of the Lagrange multiplier on the field, we get for the cumulants (at zero field)

$$C(\mu_j) = m , \quad (2.16a)$$

$$C(\mu_j\mu_k) = -N^{-1}(1-m^2) , \quad (2.16b)$$

and therefore with the aid of Table I, Eq. (2.14) becomes

$$-\beta C_1(V) = [m^2 - N^{-1}(1-m^2)]\sum_{j,k} K(j,k) . \quad (2.17)$$

At this level it would have been much easier to claim that the average $\langle \mu_j\mu_k\rangle_0$ factors, as one would expect of a noninteracting system. After all, the error introduced by doing this [which would be tantamount to neglecting the correlations induced by Eq. (2.7)] shows up only to order N^{-1} in the average and thus to order 1 in the free energy. [It will turn out that Eq. (2.16b) does contribute at the next order in Eq. (2.3), however.] In any case, concentrating for the moment on the $n=1$ level of Eq. (2.3) and on the special case of the normal Ising model of Eq. (2.6), we obtain, to order N,

$$-\beta C_1(V) = N(\beta Jz/2)m^2 ,$$

where z is the coordination number of the lattice, which, with Eq. (2.13), gives for the total free energy at zero field

$$-\beta F/N = \ln 2 - \int_0^m \tanh^{-1}x\,dx + (z\beta J/2)m^2 . \quad (2.18)$$

The magnetization can now be calculated by minimizing Eq. (2.18),

$$m = \tanh(\beta Jzm) ,$$

leading to the standard prediction for the critical temperature,[5]

$$kT_c/J = z . \quad (2.19)$$

To extend this development to Kirkwood's level of approximation we need to include the $n=2$ term in Eq. (2.3). This term can be written concisely with the aid of Eqs. (2.4) and (2.8) as

$$(2!)^{-1}(-\beta)^2 C_2(V) = (2!)^{-1}\sum_{j,k,l,m} K(j,k)K(l,m)(\langle \mu_j\mu_k\mu_l\mu_m\rangle_0 - \langle \mu_j\mu_k\rangle_0\langle \mu_l\mu_m\rangle_0) , \quad (2.20)$$

but it is convenient to evaluate it as a sum of three different types of terms: those with *two* repeated indices,

$$(2!)^{-1}2\sum_{j,k} K(j,k)K(j,k)(1-\langle \mu_j\mu_k\rangle_0^2) , \quad (2.21)$$

where the factor of 2 accounts for the equivalence of the cases $j=l$, $k=m$ and $j=m$, $k=l$; those with *one* repeated index,

TABLE I. Multisite moments in terms of multisite cumulants.

$$\begin{aligned} \langle \mu_j\rangle &= C(\mu_j) \\ \langle \mu_j\mu_k\rangle &= C(\mu_j\mu_k) + C(\mu_j)C(\mu_k) \\ &= C(\mu_j\mu_k) + C^2(\mu_j) \quad \text{(in the case of uniform order)} \\ \\ \langle \mu_j\mu_k\mu_l\rangle &= C(\mu_j\mu_k\mu_l) + C(\mu_j)C(\mu_k\mu_l) + C(\mu_k)C(\mu_j\mu_l) + C(\mu_l)C(\mu_j\mu_k) + C(\mu_j)C(\mu_k)C(\mu_l) \\ &= C(\mu_j\mu_k\mu_l) + 3C(\mu_j)C(\mu_k\mu_l) + C^3(\mu_j) \quad \text{(in the case of uniform order)} \\ \\ \langle \mu_j\mu_k\mu_l\mu_m\rangle &= C(\mu_j\mu_k\mu_l\mu_m) + C(\mu_j\mu_k)C(\mu_l\mu_m) + C(\mu_j\mu_l)C(\mu_k\mu_m) \\ &\quad + C(\mu_j\mu_m)C(\mu_k\mu_l) + C(\mu_j)C(\mu_k\mu_l\mu_m) + C(\mu_k)C(\mu_j\mu_l\mu_m) + C(\mu_l)C(\mu_j\mu_k\mu_m) + C(\mu_m)C(\mu_j\mu_k\mu_l) \\ &\quad + C(\mu_j)C(\mu_k)C(\mu_l\mu_m) + C(\mu_j)C(\mu_l)C(\mu_k\mu_m) + C(\mu_j)C(\mu_m)C(\mu_k\mu_l) + C(\mu_k)C(\mu_l)C(\mu_j\mu_m) + C(\mu_k)C(\mu_m)C(\mu_j\mu_l) \\ &\quad + C(\mu_l)C(\mu_m)C(\mu_j\mu_k) + C(\mu_j)C(\mu_k)C(\mu_l)C(\mu_m) \\ &= C(\mu_j\mu_k\mu_l\mu_m) + 3C^2(\mu_j\mu_k) + 4C(\mu_j)C(\mu_k\mu_l\mu_m) + 6C^2(\mu_j)C(\mu_k\mu_l) + C^4(\mu_j) \quad \text{(in the case of uniform order)} \end{aligned}$$

$$(2!)^{-1}4\sum_{\substack{j,k,m\\(m\neq j)}} K(j,k)K(j,m)$$
$$\times(\langle\mu_k\mu_m\rangle_0-\langle\mu_j\mu_k\rangle_0\langle\mu_j\mu_m\rangle_0)\ , \qquad (2.22)$$

where the factor of 4 accounts for the equivalence of the cases $j=l$, $j=m$, $k=l$, and $k=m$; and finally, those with *no* repeated indices,

$$(2!)^{-1}\sum_{j,k,l,m}{}' K(j,k)K(l,m)$$
$$\times(\langle\mu_j\mu_k\mu_l\mu_m\rangle_0-\langle\mu_j\mu_k\rangle_0\langle\mu_l\mu_m\rangle_0)\ , \qquad (2.23)$$

where the primed summation restricts the summation to no repeated indices. Note that expressions with three or four repeated indices would not contribute, since $K(j,j)=0$.

As before, Table I allows us to compute the necessary moments in terms of various cumulants—two of which we already have in Eqs. (2.16). Although in general one also needs $C(\mu_j\mu_k\mu_l)$ and $C(\mu_j\mu_k\mu_l\mu_m)$ in order to evaluate the fourth-order moment $\langle\mu_j\mu_k\mu_l\mu_m\rangle_0$, these two cumulants turn out to be of order N^{-2} and N^{-3}, respectively, so they are unnecessary to this order of calculation. Thus using (2.16) and Table I, we find for the sum of terms (2.21), (2.22), and (2.23), respectively (to leading order),

$$(2!)^{-1}(-\beta)^2C_2(V)=(1-m^4)\sum_{j,k}K^2(j,k)+2m^2(1-m^2)\sum_{\substack{j,k,m\\(m\neq k)}}K(j,k)K(j,m)-2N^{-1}m^2(1-m^2)\sum_{j,k,l,m}{}' K(j,k)K(l,m)\ . \qquad (2.24)$$

It is worthwhile to point out that in writing these formulas, we were able to regard $C(\mu_j\mu_k)$ as being zero (ignoring the long-range correlations) for Eqs. (2.21) and (2.22), but not for Eq. (2.23). There, the sum itself is of order N^2, so we have to keep terms of order N^{-1} in the summand.

Equations (2.13), (2.17), and (2.24), when substituted in Eq. (2.3), constitute the Kirkwood approximation for the most general Ising-like Hamiltonian, Eq. (2.5), providing we assume uniform ordering. If we again specialize to the normal Ising model though, Eq. (2.24) reduces to

$$(2!)^{-1}(-\beta)^2C_2(V)=N(\beta J/2)^2z(1-m^2)^2\ ,$$

and on appending it to Eq. (2.18), one gets for the free energy

$$-\beta F/N=\ln 2-\int_0^m \tanh^{-1}x\,dx$$
$$+(\beta J/2)zm^2+(\beta J/2)^2z(1-m^2)^2\ . \qquad (2.25)$$

The magnetization in the Kirkwood approximation must therefore satisfy the minimum condition

$$m=\tanh[(\beta J)zm-(\beta J)^2zm(1-m^2)]\ , \qquad (2.26)$$

from which the critical temperature may be determined by solving the quadratic equation

$$(\beta_cJ)z-(\beta_cJ)^2z=1\ ,$$

leading to

$$kT_c/J=z[1+(1-4z^{-1})^{1/2}]/2\ . \qquad (2.27)$$

To gauge the improvement we have obtained by including the first fluctuation term in Eq. (2.3) (taking ordinary mean-field theory into the Kirkwood approximation), we can compare the critical temperatures predicted for a simple-cubic lattice in three dimensions ($z=6$). The ordinary mean-field temperature, Eq. (2.19), is

$$kT_c/J=6\ ,$$

and the Kirkwood result, Eq. (2.27), is

$$kT_c/J=3+\sqrt{3}=4.731\ ,$$

whereas the "exact" result from series expansion[31] is

$$kT_c/J=4.511\ .$$

Hence the Kirkwood method does indeed take into account the way in which fluctuations depress the critical point (see Fig. 1).[32] In particular, unlike the Bragg-Williams theory, the improved method correctly predicts that one dimensional systems ($z=2$) have no finite-temperature transition, although it incorrectly predicts that the two-dimensional hexagonal lattice ($z=3$) also does not have a transition. Presumably this approach is not as good in two dimensions as it is in three (where fluctuations play a less dominant role). However, the success in three dimensions (3D) gives us some confidence that the approach will be able to help us in the next section when we study the influence of fluctuations in the 3D ANNNI model.

B. A modulated system: The ANNNI model

In this section we want to extend the results of Sec. II A for uniformly ordered systems so as to be able to study the effect of fluctuations on more complicated orderings. As we have previously suggested, our generalization does not involve a change in the Hamiltonian of Eq. (2.8), and consequently does not invalidate the free-energy expansion encompassed by Eqs. (2.3), (2.14), and (2.20). It simply requires us to replace the single order parameter defined by Eq. (2.7) with a *set* of order parameters and to compute the necessary cumulants in terms of these new order parameters.

A convenient framework for this calculation is provided by breaking the system up into sublattices, each of which has a distinct order parameter. At a very simple level, this same idea is used to treat the Ising antiferromagnet.[22] There one divides the lattice in advance into

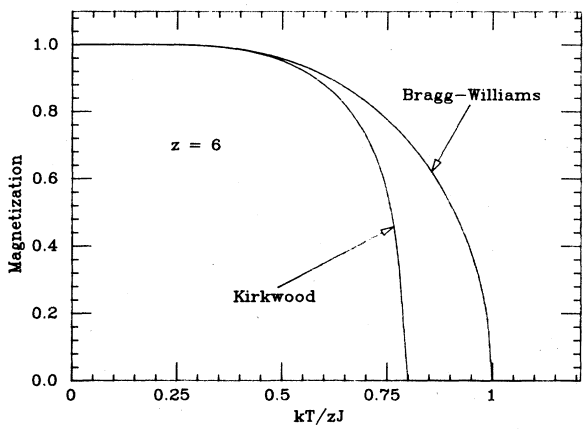

FIG. 1. Magnetization of an Ising ferromagnet on a simple-cubic lattice vs temperature. The Bragg-Williams and Kirkwood approximations are shown, plotted as m vs T in units of zJ/k, where z is the coordination number of the lattice and J is the coupling constant. Notice how the magnetization in the Kirkwood approximation is always less than or equal to the Bragg-Williams result.

two interpenetrating sublattices such that each site is on a different sublattice than its nearest neighbors. Of course, for the antiferromagnet one knows that the form of the ordered state is consistent with this division. Not having any such foreknowledge in general, we will have to break up the N-site lattice formally into n sublattices, denoted S_α $(\alpha=1,\ldots,n)$. Each sublattice is disjoint from the others and is assumed to contain a macroscopic number of sites N_α so that

$$\sum_{\alpha=1}^{n} N_\alpha = N \ .$$

Fortunately, the physical location of the sublattices need not be specified at this stage, but it is clear that this kind of approach will only prove useful if the sublattices turn out to be uniformly ordered themselves. In principle, this requirement could be translated into necessary and sufficient conditions for the permissible interactions $K(j,k)$ between sites j and k as a function of which sublattice(s) j and k are in. However, such a translation is tantamount to solving the highly nontrivial problem of prescribing what characteristics a Hamiltonian has to have to generate modulated order. We will eschew any real attempt in this direction here, though we will impose the physically similar requirement that the interaction between the spins on any two given sublattices, α and β (whether α and β are the same or not), involves only one energy scale. That is, we can define a set of constants $J_{\alpha\beta}$ such that

$$K(j,k)=0 \ \text{ or } \ \beta J_{\alpha\beta}/2$$

if $j\in S_\alpha$ and $k\in S_\beta$, regardless of the exact location of j and k.

With this proviso, we can introduce a separate magnetization for each sublattice,

$$m_\alpha = N_\alpha^{-1} \sum_{\substack{i \\ (i\in S_\alpha)}} \mu_i \ , \tag{2.28}$$

giving for the reference free energy analogous to Eq. (2.11)

$$-\beta F_0(m_1,\ldots,m_n) = \sum_{\alpha=1}^{n} \left[-\lambda_\alpha N_\alpha m_\alpha + \sum_{\substack{j \\ (j\in S_\alpha)}} \ln\{2\cosh[h(j)+\lambda_\alpha]\} \right] , \tag{2.29}$$

with the, now, n λ_α's determined by the n equations

$$\sum_{\substack{j \\ (j\in S_\alpha)}} \tanh[h(j)+\lambda_\alpha] = N_\alpha m_\alpha \ . \tag{2.30}$$

Then, as before, the multisite cumulants can be derived by using Eq. (2.29) as a generating function. In particular, the analogs of Eqs. (2.16) are

$$C(\mu_j) = m_\alpha \ , \tag{2.31a}$$

$$C(\mu_j\mu_k) = -N_\alpha^{-1}(1-m_\alpha^2)\delta_{\alpha\beta} \ , \tag{2.31b}$$

where $\mu_j\in S_\alpha$, $\mu_k\in S_\beta$, and $\delta_{\alpha\beta}$ is the Kronecker delta ($\delta=1$ if $\alpha=\beta$, 0 if $\alpha\neq\beta$). Note that cumulants contribute only if all the μ's are on the same sublattice (because there is no correlation between the sublattices).

Equations (2.29)—(2.31) are enough to enable us to evaluate the zeroth- and first-order terms in Eq. (2.3)—the Bragg-Williams mean-field theory. Using Eq. (2.14) implies that (ignoring terms of order N_α^{-1})

$$-\beta C_1(V) = \sum_{\alpha=1}^{n} \sum_{\substack{j \\ (j\in S_\alpha)}} \sum_{\beta=1}^{n} \sum_{\substack{k \\ (k\in S_\beta)}} K(j,k)\langle\mu_j\mu_k\rangle_0 = \sum_{\alpha,\beta=1}^{n} \tilde{K}(\alpha,\beta) m_\alpha m_\beta \ ,$$

where

$$\tilde{K}(\alpha,\beta) \equiv \sum_{\substack{j \\ (j\in S_\alpha)}} \sum_{\substack{k \\ (k\in S_\beta)}} K(j,k) \tag{2.32}$$

so that, the Bragg-Williams free energy for zero field is

$$-\beta F = N\ln 2 - \sum_{\alpha=1}^{n} \int_0^{m_\alpha} \tanh^{-1}x \, dx + \sum_{\alpha,\beta=1}^{n} \tilde{K}(\alpha,\beta) m_\alpha m_\beta \ . \tag{2.33}$$

The magnetizations are therefore the solution of a set of coupled nonlinear equations

$$m_\alpha = \tanh\left[\sum_{\beta=1}^{n} \tilde{K}(\alpha,\beta) m_\beta \right] \quad (\alpha=1,\ldots,n) \ . \tag{2.34}$$

Unlike the superficially very similar case of a uniform system ($n=1$), these equations will usually have a very

large number of roots, making the necessary multidimensional root search reasonably difficult.

To apply this fully general theory, we have to specify the interactions in more detail. Accordingly, just as we used the Ising model as an example in Sec. II A, let us consider the three-dimensional ANNNI model as an example here. The model consists of Ising spins on a simple-cubic lattice with interactions[2]

$$K(j,k)=\beta J_0/2 \quad (J_0>0)\,, \tag{2.35a}$$

if j and k are nearest neighbors in the x-y plane,

$$K(j,k)=\beta J_1/2 \quad (J_1>0) \tag{2.35b}$$

if j and k are nearest neighbors in the z direction, and

$$K(j,k)=\beta J_2/2 \quad (J_2<0) \tag{2.35c}$$

if j and k are next-nearest neighbors in the z direction. Otherwise, the interactions vanish. Because of the way in which the interactions are arranged, the modulation occurs only along the z axis, which suggests that each x-y plane be considered a different sublattice. If we do so, Eqs. (2.33) and (2.34) become

$$-\beta F/N=\ln 2-n^{-1}\sum_{\alpha=1}^{n}\Big[\int_0^{m_\alpha}\tanh^{-1}x\,dx-2\beta J_0 m_\alpha^2 -(\beta J_1/2)m_\alpha(m_{\alpha+1}+m_{\alpha-1}) -(\beta J_2/2)m_\alpha(m_{\alpha+2}+m_{\alpha-2})\Big], \tag{2.36}$$

$$m_\alpha=\tanh\beta[4J_0 m_\alpha+J_1(m_{\alpha+1}+m_{\alpha-1}) +J_2(m_{\alpha+2}+m_{\alpha-2})]\,. \tag{2.37}$$

These equations are precisely the ANNNI mean-field theory that has already been extensively studied in the literature. The only exact analytical result available from Eq. (2.37) is the temperature at which ordering first occurs,[1] but numerical studies have revealed a rich structure at somewhat lower temperatures. Most notably Bak and von Boehm[2] and Yokoi, Coutinho-Filho, and Salinas[3]

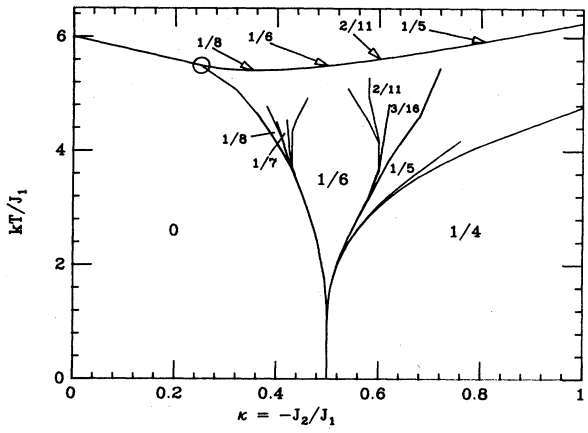

FIG. 2. Phase diagram of the ANNNI model in the Bragg-Williams approximation, plotted as reduced temperature vs the ratio of antiferromagnetic to ferromagnetic coupling. The numbers $\frac{1}{4},\frac{1}{5},\frac{1}{6},\ldots$ are the wave numbers q of the various modulated phases. Thus $q=0$ corresponds to the ferromagnetic region. The critical line between the paramagnetic and ordered regions is marked by arrows indicating the points at which the regions associated with some selected phases terminate. Note also the position of the Lifshitz point (circled). Near this critical line, the value of q varies continuously, so the assumption of an integral periodicity (which we used to calculate the diagram) breaks down. We have therefore not extended our phases boundaries up to the line. As with Ref. 2, we have labeled each phase with the q value of its largest Fourier component.

have used the method mentioned in the Introduction of decoupling Eq. (2.37) by assuming modulated structures of finite periodicity P. For purposes of comparison with what is to come, we have reconstructed the Bak and von Boehm phase diagram in Fig. 2, extending their calculation to P as high as 20.

Continuing the analogy with Sec. II A, the next step is to go to higher order in Eq. (2.3): to implement the Kirkwood approximation for modulated order by evaluating Eqs. (2.20). Rewriting this fluctuation term as a sum over sublattices gives

$$(2!)^{-1}(-\beta)^2 C_2(V)=(2!)^{-1}\sum_{\alpha,\beta,\gamma,\delta=1}^{n}\sum_{j\in S_\alpha}\sum_{k\in S_\beta}\sum_{l\in S_\gamma}\sum_{m\in S_\delta}K(j,k)K(l,m)F(j,k,l,m)\,, \tag{2.38}$$

where

$$F(j,k,l,m)\equiv\langle\mu_j\mu_k\mu_l\mu_m\rangle_0-\langle\mu_j\mu_k\rangle_0\langle\mu_l\mu_m\rangle_0 \tag{2.39}$$

can be calculated by using Table I and Eq. (2.31), at least through order N_α^{-1}. Note that F vanishes unless the pairs j,k and l,m are connected in the sense that they have at least one sublattice in common.

This latter observation suggests that it may be helpful to partition the sums in Eq. (2.38) further with respect to the degree of sublattice connectivity,

$$\sum_{\alpha,\gamma=1}^{n}\sum_{\substack{j\\(j\in S_\alpha)}}\sum_{\substack{k\\(k\in S_\gamma)}}\sum_{\substack{l\\(l\in S_\gamma)}}\sum_{\substack{m\\(m\in S_\alpha)}}K(j,k)K(l,m)F(j,k,l,m)+\sum_{\alpha=1}^{n}\sum_{\substack{\beta\\(\beta\neq\alpha)}}^{n}\sum_{\substack{j\\(j\in S_\alpha)}}\sum_{\substack{k\\(k\in S_\beta)}}\sum_{\substack{l\\(l\in S_\alpha)}}\sum_{\substack{m\\(m\in S_\beta)}}K(j,k)K(l,m)F(j,k,l,m)$$
$$+\sum_{\alpha=1}^{n}\sum_{\substack{\gamma\\(\gamma\neq\alpha)}}^{n}\sum_{\substack{\beta\\(\beta\neq\gamma)}}^{n}\sum_{\substack{j\\(j\in S_\alpha)}}\sum_{\substack{k\\(k\in S_\beta)}}\sum_{\substack{l\\(l\in S_\gamma)}}\sum_{\substack{m\\(m\in S_\beta)}}K(j,k)K(l,m)F(j,k,l,m)$$
$$+\sum_{\alpha,\gamma}^{n}\sum_{\substack{\beta\\(\beta\neq\gamma)}}^{n}\sum_{\substack{\delta\\(\delta\neq\alpha,\beta)}}^{n}\sum_{\substack{j\\(j\in S_\alpha)}}\sum_{\substack{k\\(k\in S_\beta)}}\sum_{\substack{l\\(l\in S_\gamma)}}\sum_{\substack{m\\(m\in S_\delta)}}K(j,k)K(l,m)F(j,k,l,m)\,. \tag{2.40}$$

Indeed, it turns out that only the first two terms of Eq. (2.40) yield nonzero results. (For proof, the reader is referred to the Appendix). Thus, the final, fully general result for the first fluctuation correction to the mean-field theory of modulated order is

$$(2!)^{-1}(-\beta)^2 C_2(V)=(2!)^{-1}\sum_{\alpha=1}^{n}\left[\sum_{j,k,l,m\in S_\alpha} K(j,k)K(l,m)F(j,k,l,m)+2\sum_{\substack{\gamma\\(\gamma\neq\alpha)}}\sum_{\substack{j,m\in S_\alpha\\k,l\in S_\gamma}} K(j,k)K(l,m)F(j,k,l,m)\right], \tag{2.41}$$

where F is defined by Eq. (2.39), Table I, and Eq. (2.31). Although it is difficult to read much into Eq. (2.41) without explicitly defining the interactions, it is worth pointing out that even at this level, the form of the equation is indicative of a feedback or polarization effect (an Onsager reaction field[33]). Remembering that $K(j,k)$ can always be written as some $\beta J_{\alpha\gamma}/2$ tells us that only feedback terms such as $J_{\alpha\gamma}^2$ show up in Eq. (2.41): sublattice α affects sublattice γ which, in turn, affects sublattice α. Cross terms such as $J_{\alpha\beta}J_{\gamma\delta}$ do not appear.

We are now, finally, ready to apply all of the ideas of this paper to the ANNNI model. With the aid of Eq. (2.35) we find the Kirkwood approximation to the ANNNI free energy by adding Eq. (2.41) to Eq. (2.36),

$$-\beta F/N=\ln 2-n^{-1}\sum_{\alpha=1}^{n}\int_0^{m_\alpha}\tanh^{-1}x\,dx+\beta n^{-1}\sum_{\alpha=1}^{n}(2J_0m_\alpha^2+J_1m_\alpha m_{\alpha+1}+J_2m_\alpha m_{\alpha+2})$$
$$+\beta^2(2!)^{-1}n^{-1}\sum_{\alpha=1}^{n}[2J_0^2(1-m_\alpha^2)^2+J_1^2(1-m_\alpha^2)(1-m_{\alpha+1}^2)+J_2^2(1-m_\alpha^2)(1-m_{\alpha+2}^2)]\,. \tag{2.42}$$

When minimized, this free energy gives us the desired coupled set of equations for the layer magnetizations,

$$m_\alpha=\tanh[4\beta J_0m_\alpha+\beta J_1(m_{\alpha+1}+m_{\alpha-1})+\beta J_2(m_{\alpha+2}+m_{\alpha-2})-4(\beta J_0)^2m_\alpha(1-m_\alpha^2)$$
$$-(\beta J_1)^2m_\alpha(2-m_{\alpha+1}^2-m_{\alpha-1}^2)-(\beta J_2)^2m_\alpha(2-m_{\alpha+2}^2-m_{\alpha-2}^2)]\,. \tag{2.43}$$

As with the previously derived, lower-level mean-field theory, Eqs. (2.36) and (2.37), it is possible to locate the second-order-transition line analytically (that is, to find the line between the disordered high-temperature phase and the ordered low-temperature phases analytically). Near the critical temperature T_c we can linearize Eq. (2.43), yielding a set of coupled difference equations

$$m_\alpha=4\beta J_0m_\alpha+\beta J_1(m_{\alpha+1}+m_{\alpha-1})+\beta J_2(m_{\alpha+2}+m_{\alpha-2})$$
$$-[4(\beta J_0)^2+2(\beta J_1)^2+2(\beta J_2)^2]m_\alpha$$

which can then be decoupled into separate equations for the Fourier components of the magnetization, m_q,

$$m_q=\{4\beta J_0+2\beta J_1\cos(2\pi q)+2\beta J_2\cos(4\pi q)$$
$$-[4(\beta J_0)^2+2(\beta J_1)^2+2(\beta J_2)^2]\}m_q\,, \tag{2.44}$$

where, in standard notation,[3]

$$m_q=\sum_\alpha e^{2\pi iq\alpha}m_\alpha\,.$$

Let us adopt the standard definition of the ratio of the antiferromagnetic to the ferromagnetic interaction,

$$\kappa\equiv -J_2/J_1\,, \tag{2.45}$$

and make the standard assumption that $J_0=J_1$. The critical line can now be specified by finding the maximum temperature such that the brace on the right-hand side of Eq. (2.44) equals 1. If $\kappa>\frac{1}{4}$, maximizing the temperature give us the same critical wave number q_c as the Bragg-Williams theory,

$$\cos(2\pi q_c)=J_1/4J_2=(4\kappa)^{-1}\,, \tag{2.46}$$

TABLE II. Critical temperature of the ANNNI model.

κ	T_c (Bragg-Williams)[a]	T_c (Kirkwood)[b]	T_c (Monte Carlo)	T_c (series)
0.100	5.800	4.446	4.20±0.02[c]	4.24±0.02[e]
0.250	5.500	3.949	3.80±0.02[c]	3.78±0.02[e]
0.271	5.458	3.880	3.70±0.02[c]	3.72±0.02[e]
0.600	5.617	3.880	3.82±0.03[d]	3.82±0.02[f]

[a]Standard mean-field theory, Ref. 1 (all temperatures are in units of J_1/k).
[b]The present work.
[c]Monte Carlo data from Ref. 10(a).
[d]Monte Carlo, with finite-size scaling corrections, from Ref. 10(b).
[e]High-temperature-series expansion of S. Redner and H. E. Stanley [Phys. Rev. B **11**, 133 (1978); J. Phys. C **10**, 4765 (1977)], as quoted in Ref. 10(a).
[f]Redner and Stanley, quoted in Ref. 10(b).

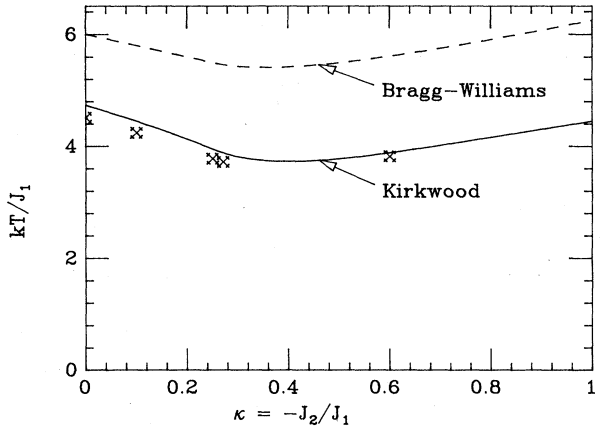

FIG. 3. Critical line for the ANNNI model in the Bragg-Williams and Kirkwood approximations, plotted as reduced temperature vs κ. The starred points are accurate high-temperature-series results. All but the $\kappa=0$ point are from Ref. 10. The $\kappa=0$ point is the pure Ising result given in Ref. 31.

but leads to a lower critical temperature,

$$kT_c/J_1=\kappa^{-1}\{\kappa^2+2\kappa+\tfrac{1}{8}+[-\kappa^4+4\kappa^3-(\tfrac{7}{4})\kappa^2+\tfrac{1}{2}\kappa+\tfrac{1}{64}]^{1/2}\}\ . \quad (2.47)$$

If $\kappa<\frac{1}{4}$, the critical wave number is zero (i.e., the ordered phase is no longer modulated) and the critical temperature is simply

$$kT_c/J_1=3-\kappa+(3-6\kappa-\kappa^2)^{1/2}\ . \quad (2.48)$$

This transition point along the critical line, marking the coexistence of paramagnetic, ferromagnetic, and modulated phases, is commonly called the Lifshitz point.[34] It is worth noting that the Kirkwood approximation locates this point at

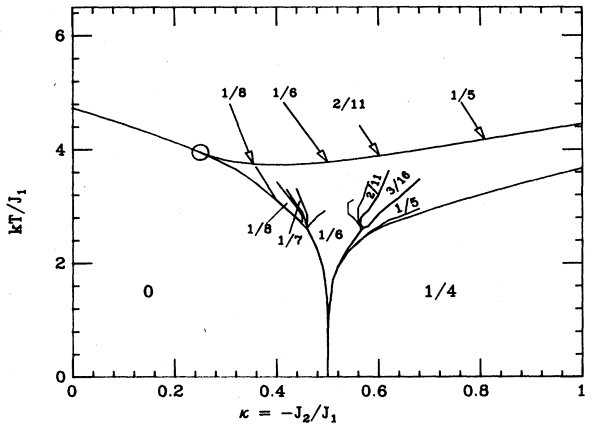

FIG. 4. Phase diagram of the ANNNI model in the Kirkwood approximation using the same notation as Fig. 2. Comparison with Fig. 2 reveals both that the disordered region starts at a significantly lower temperature and that the extent of the higher-order commensurate phases (the "fan") is reduced in this figure.

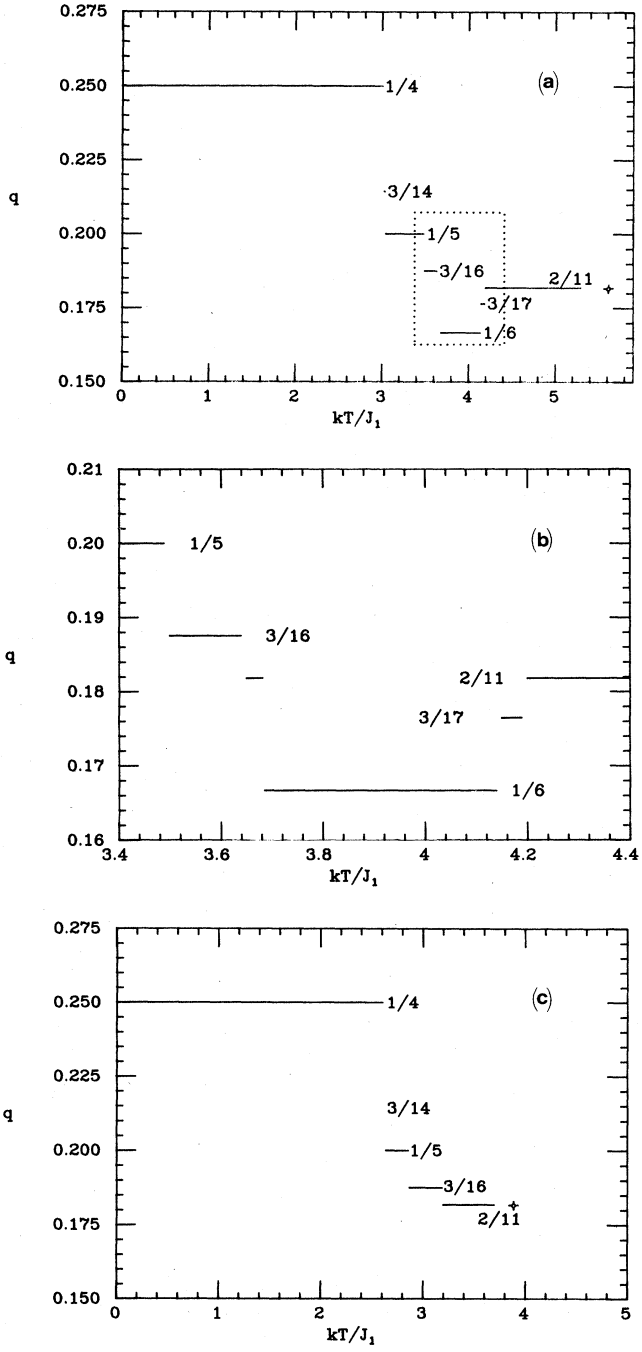

FIG. 5. Wave number q of the equilibrium ANNNI phases as a function of reduced temperature, for fixed $\kappa=0.60$. In (a) the Bragg-Williams solution is presented (corresponding to a vertical slice through Fig. 2). The dotted rectangle is expanded in (b) to show the reentrant behavior of $q(T)$ for the $q=\frac{2}{11}$ and $\frac{3}{17}$ phases. See Ref. 36 in this connection. In the Kirkwood approximation, (c) (corresponding to Fig. 4), no reentrant behavior is seen for this choice of κ. Note, however, that the value of κ was chosen so as to permit comparison with Refs. 3 and 10, and that other choices would indeed show reentrant behavior in the Kirkwood approximation, though to a greatly reduced extent than in the Bragg-Williams. The star in the figures marks the critical wave number and temperature.

$$\kappa=\tfrac{1}{4},\quad kT_c/J_1=(11+\sqrt{23})/4\cong 3.9490\ ,$$

which is also at the same κ, but at a lower temperature than the result of the lower-order mean-field theory ($kT_c/J_1=\frac{11}{2}$). For completeness, we note that the Bethe approximation of Taylor and Desjardins leads to a numerical estimate of $\kappa\sim 0.27$ at the Lifshitz point.[23] In Table II and Fig. 3 we make a more extensive comparison of our results for the critical line with the results from the literature.

The remainder of our predicted phase diagram, calculated numerically[35] from Eqs. (2.42) and (2.43), is shown in Fig. 4. By comparing it with Fig. 2 we observe that the diagrams are qualitatively similar, but there are nonetheless pronounced quantitative differences. Most obviously, the entire ordered region becomes smaller when fluctuations are included—T_c is lowered just as it was for the Ising model. But, in addition, *within* the ordered region, the portion occupied by the high-order modulated phases has shrunken noticeably. For example, the $q=\frac{1}{6}$ region spans a range in κ of only ~ 0.10 as compared with ~ 0.15 in lower-order mean-field theory. Apparently, modulated phases are more susceptible to destruction by fluctuations than are more conventionally ordered phases. Furthermore, considering just these modulated phases, we also see that reentrant behavior is suppressed by fluctuations (as shown in greater detail in Fig. 5). That is, there is less likelihood of encountering the same phase twice as one increases temperature at constant κ (proceeds vertically in Figs. 2 or 4). This result is consistent with what had been observed previously in the case of the Ising antiferromagnet[37] and in Monte Carlo studies of the ANNNI model itself.[10(b)]

Before discussing these findings in any depth, as we will do in the next section, there is still a final point worth making. The analogies between the models of modulated order and spin glasses that we alluded to in the Introduction have largely been physical, not computational. Thus it is somewhat surprising to find that the Kirkwood self-consistent equations for the magnetization, Eq. (2.43), are precisely the Thouless-Anderson-Palmer (TAP) equations[25]

$$m_i=\tanh\left[\sum_j \beta J_{ij}m_j-m_i\sum_j(\beta J_{ij})^2(1-m_j^2)\right]$$

used in studying spin glasses.

III. DISCUSSION

Probably the most important general contribution of this paper was to extend the mean-field theory of modulated order to the Kirkwood level of approximation, Eq. (2.41). With this extension (and the systematic inclusion of higher-order terms in the free-energy-cumulant expansion, if desired) one is now free to study at least some of the effects of fluctuations on modulated structures. It should be noted that the analogous cluster-variation, or Bethe, method, had already been so extended,[23,24] but we find (as did Kirkwood himself[20]) that the Kirkwood method is both somewhat easier to apply and interpret and slightly more accurate.[22,32,38]

Almost as important as this general result was the specific application to the ANNNI model, Eqs. (2.42) and (2.43). Here again the Kirkwood method pays a bonus in enabling us not only to calculate the phase diagram but also to understand the results physically. Consider the effective (mean) magnetic field implied by ordinary mean-field theory, Eq. (2.37),

$$4(\beta J_0)m_\alpha+(\beta J_1)(m_{\alpha+1}+m_{\alpha-1})+(\beta J_2)(m_{\alpha+2}+m_{\alpha-2})\ , \tag{3.1}$$

and the fluctuation correction to it in Eq. (2.43),

$$-4(\beta J_0)^2m_\alpha(1-m_\alpha^2)-(\beta J_1)^2m_\alpha(2-m_{\alpha+1}^2-m_{\alpha-1}^2)$$
$$-(\beta J_2)^2m_\alpha(2-m_{\alpha+2}^2-m_{\alpha-2}^2)\ . \tag{3.2}$$

Independently of any of the details, the overall minus sign in Eq. (3.2) means that fluctuations always diminish the *magnitude* of the effective field. Hence, as has long been known, the ordered region will always be suppressed by fluctuations, regardless of whether there are modulations or not. However, in looking at Eq. (3.1) in more detail, we see that modulated structures exist only because the effective-field mimics, or is coherent with, the modulation. The positive J_1 term favors alignment with nearest neighbors ($\alpha\pm 1$), whereas the negative J_2 term favors antialignment with the next-nearest neighbors. Thus when the fluctuation term is added—with the J_1 and J_2 terms both coming in with the same sign—one finds that fluctuations must also diminish the *coherence* of the effective field. Consequently, the width of the highly modulated region shrinks, just as we observed in the preceding section.

The final major result of this paper, the emergence of the TAP equations[25] in a context apparently not involving random magnets, is difficult to discuss at this stage. Indeed, although there are similarities between the phase diagrams of the ANNNI and spin-glass models[17] and although there is a certain amount of nonergodicity in the numerical treatment of the ANNNI model,[16] the two systems nonetheless seem to be very different. Appropriately enough, a few of these differences actually showed up in our derivation of the TAP equations.

For example, although both approaches needed to consider some sort of order-parameter function, the function introduced here was the magnetization as a function of *sublattice*. Unlike the TAP equation, in which each spin functioned as its own sublattice, we were forced to assume sublattices of macroscopic extent. On the other hand, we were not required to introduce an infinitely weak, infinitely long-range potential. The practical result was that we discarded terms of order N^{-1}, whereas TAP theory neglects terms of order Z^{-1} (Z being the interaction range).[26]

These very distinctions, however, permit us to point out a few basic features of the TAP equations which are difficult to see when the equations are viewed solely in their traditional spin-glass setting.[26] First of all, the fluctuation term which differentiates TAP theory from ordinary mean-field theory can be important whether the equations are applied to spin glasses or not. Certainly the removal

of the predicted transition in one dimension is a fundamental qualitative feature. Secondly, the order-N^{-1} terms which have to be kept in deriving the fluctuation correction are also not unique to spin glasses, nor are they unique to the use of a weak, long-range potential. Rather they are a natural consequence of the system-wide correlations introduced by fixing an order parameter. Finally, the TAP equations are more closely connected with the Kirkwood approximation than they are with the Bethe. Thus, any worry about how to think about spin-glass frustation on a lattice with no loops[26] would seem to be irrelevant

Further connections between random magnets and systems with modulated order will, unfortunately, have to wait until the following paper.[4] For the time being though, it probably suffices to emphasize our main point: that it is both possible and useful to study the effect of fluctuations, even far from critical points, when nontrivial ordering is involved.

ACKNOWLEDGMENT

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APPENDIX

The purpose of this appendix is to show that Eq. (2.40) reduces to Eq. (2.41); specifically, that the last two terms in Eq. (2.40) vanish.

First, notice that the factor $F(j,k,l,m)$ vanishes if all the indices are on different sublattices, for if there are no repeated indices, $F(j,k,l,m)$ is given by (to leading order in N_α^{-1})

$$C(\mu_j)C(\mu_l)C(\mu_k\mu_m)+C(\mu_j)C(\mu_m)C(\mu_k\mu_l) + C(\mu_k)C(\mu_l)C(\mu_j\mu_m)+C(\mu_k)C(\mu_m)C(\mu_j\mu_l)\ , \tag{A1}$$

which is nonzero only if at least one pair of indices appearing in a multisite cumulant are on the same sublattice [see Eq. (2.31)]. In evaluating (2.40), we therefore need only consider cases where at least one of the pairs

$$\alpha,\gamma \quad \alpha,\delta \quad \beta,\gamma \quad \beta,\delta$$

involves only one sublattice.

With this in mind, we can write the contribution from the *last* term in Eq. (2.40) as

$$\sum_{\alpha=\gamma=1}^{n} \sum_{\substack{\beta \\ (\beta\neq\alpha)}}^{n} \sum_{\substack{\delta \\ (\delta\neq\alpha,\beta)}}^{n} \sum_{\substack{j \\ (j\in S_\alpha)}} \sum_{\substack{k \\ (k\in S_\beta)}} \sum_{\substack{l \\ (l\in S_\alpha)}} \sum_{\substack{m \\ (m\in S_\delta)}} K(j,k)K(l,m)F(j,k,l,m)\ , \tag{A2}$$

since only if $\alpha=\gamma$ can we have a contribution. Here we have the possibility of a repeated index, in which case $F(j,k,l,m)$ is given, not by Eq. (A1), but by (again to leading order)

$$C(\mu_k)C(\mu_m)[1-C(\mu_j)C(\mu_l)]=m_\beta m_\delta(1-m_\alpha^2)\ . \tag{A3}$$

If there are no repeated indices, Eq. (A1) applies, and, with only j and l on the same sublattice, the value of $F(j,k,l,m)$ is

$$-N_\alpha^{-1}m_\beta m_\delta(1-m_\alpha^2)\ . \tag{A4}$$

With Eqs. (A3) and (A4), Eq. (A2) becomes

$$\sum_{\alpha=1}^{n} \sum_{\substack{\beta \\ (\beta\neq\alpha)}}^{n} \sum_{\substack{\delta \\ (\delta\neq\alpha,\beta)}}^{n} \left[-N_\alpha^{-1}m_\beta m_\delta(1-m_\alpha^2) \sum_{\substack{j \\ (j\in S_\alpha)}} \sum_{\substack{k \\ (k\in S_\beta)}} \sum_{\substack{l \\ (l\in S_\alpha)}}{}' \sum_{\substack{m \\ (m\in S_\delta)}} K(j,k)K(l,m) \right.$$

$$\left. +m_\beta m_\delta(1-m_\alpha^2) \sum_{\substack{j \\ (j\in S_\alpha)}} \sum_{\substack{k \\ (k\in S_\beta)}} \sum_{\substack{m \\ (m\in S_\delta)}} K(j,k)K(j,m) \right]\ , \tag{A5}$$

where the prime on the l sum means the $l=j$ term is excluded.

Now, if the value of the interaction depends only on the sublattice indices, as we stated in Sec. II, the sum on l in Eq. (A5) can be replaced by a factor $N_\alpha K(j,m)$, because

$$\sum_{\substack{j \\ (j\in S_\alpha)}} \sum_{\substack{l \\ (l\in S_\alpha)}}{}' K(j,k)K(l,m) = (N_\alpha-1) \sum_{\substack{j \\ (j\in S_\alpha)}} K(j,k)K(j,m)\ .$$

(The sum on j properly counts the coordination number.)

With this result, we see that Eq. (A5), which is all that is left of the contribution from the last line of Eq. (2.40), vanishes.

To arrive at our desired result, Eq. (2.41), we now only need to show that the *third* term of Eq. (2.40) vanishes also. As this term is defined, $\beta=\delta$, but α may, or may not, equal β. If $\alpha\neq\beta$ we are back to Eq. (A2) (exactly one repeated sublattice index) so, by the same argument as above, there is no contribution. In the case of $\alpha=\beta$, both j,m and k,m are on the same sublattice; there are now *two* ways to get one repeated index. Also, *two* terms in Eq. (A1) contribute, so that, just as in Eq. (A5), the contribution from terms with two repeated indices cancels with that from terms with one repeated index.

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