Journal of Statistical Physics, Vol. 51, Nos. 3/4, 1988

Modulated Phases and the Mean-Field Theory of Magnetism with Competing Interactions

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Received July 23, 1987; revision received February 2, 1988

The mean-field theory of an Ising magnet with infinitely weak, infinitely long-range potentials of arbitrary sign is presented in terms of a variational principle for the magnetization. Previous studies of the theory have revealed paramagnetic, ferromagnetic, and modulated phases. For a particular choice of potential, which is an obvious continuous version of the between-plane ANNNI model interaction, exact solutions of the stationary condition implied by the variational principle are obtained. This leads us to formulate a trial magnetization to well describe the modulated phase in general. To illustrate the utility of the trial magnetization, both analytic and numerical calculations are performed, which determine the wavenumber in certain portions of the modulated phase for the above-mentioned potential.

KEY WORDS: Mean-field theory; variational principle; modulated phase; ANNNI model.

1. INTRODUCTION

Throughout the development of statistical mechanics, mean-field theory has been of both practical utility and theoretical firmness. The mean-field approximation often predicts qualitatively correct information regarding the phase diagram of a model system, thus providing a theoretical prediction with which to compare experimental data. On the other hand, much is known rigorously under what conditions the mean-field theory can be exact.

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One such rigorous result is that of Lebowitz and Penrose.[1] They showed that the van der Waals mean-field theory is exact for infinitely weak, infinitely long-range potentials of the Kac type

$$-\gamma^{\nu} V(\gamma \mathbf{r}) \tag{1.1}$$

where one takes $\gamma \to 0^+$ after the thermodynamic limit. As well as an integrability constraint on V, one of the key conditions is that V be everywhere positive (purely attractive potential). Gates and Penrose[2] investigated the case where this latter condition is relaxed. They found that if V is such that its Fourier transform

$$\hat{V}(\mathbf{u}) = \int_{\mathbf{R}^d} d\mathbf{x}\, V(\mathbf{x}) \exp(2\pi i \mathbf{x} \cdot \mathbf{u}) \tag{1.2}$$

has its maximum for some $\mathbf{u} \neq \mathbf{0}$, then the van der Waals theory is violated.

Related to this result is the experimentally comparable mean-field calculation of the phase diagram of the axial next-nearest neighbor Ising (ANNNI) model[3,4] (see refs. 4 for review). In the three-dimensional case, on a simple cubic lattice, the original model consists simply of ferromagnetic nearest neighbor interactions $J_0 > 0$ within planes. However, between planes there are both nearest neighbor ferromagnetic couplings, $J_1 > 0$, and next-nearest neighbor antiferromagnetic couplings, $J_2 = -\kappa J_1 < 0$. A mean-field theory is constructed by neglecting the fluctuations in the layer magnetizations. This leads to a one-dimensional local mean-field theory, with couplings between the nearest and next-nearest mean layer magnetizations. As κ increases, the Fourier transform of the potential exhibits a maximum at nonzero u. The theory predicts three phases: paramagnetic, ferromagnetic, and modulated, separated by a Lifschitz point. The modulated phase itself contains an infinity of phases, which can be broadly categorized as having wavenumber commensurate or incommensurate with the lattice spacing.

An obvious problem is presented: connect up these two studies to develop an exact mean-field theory of magnetic systems with competing interactions. This task was initiated in the first paper of this series.[5]

Consider a one-dimensional Ising model of N spins μ_i, $i = 1, 2,..., N$, with interaction energy

$$E\{\mu\} = -\sum_{1 \leqslant i < j \leqslant N} \gamma V(\gamma\, |i - j|)\, \mu_i \mu_j \tag{1.3}$$

and assume only that $V(x)$ is symmetric, bounded, and Riemann-integrable over any subinterval of the real line. Then in the mean-field limit ($\gamma \to 0^+$

following the thermodynamic limit) the free energy ψ is given by the variational principle[5]

$$-\beta\psi = \max_{\{m(x)\}} \lim_{M \to \infty} f_M\{m(x)\} \tag{1.4}$$

The $m(x)$, which are magnetizations, have the restriction

$$-1 \leqslant m(x) \leqslant 1 \tag{1.5}$$

and the functional f_M is defined by

$$f_M\{m(x)\} = E_1\{m(x)\} + E_2\{m(x)\} \tag{1.6}$$

where

$$E_1\{m(x)\} = (4M)^{-1} \beta \iint_{-M}^{M} dx\, dy\, V(|x-y|)\, m(x)\, m(y) \tag{1.7}$$

$$E_2\{m(x)\} = -(2M)^{-1} \int_{-M}^{M} dx \left[\frac{1+m(x)}{2} \log\left(\frac{1+m(x)}{2}\right) + \frac{1-m(x)}{2} \log\left(\frac{1-m(x)}{2}\right)\right] \tag{1.8}$$

The condition for an extremum implies the nonlinear integral equation

$$m(x) = \tanh\left[\beta \int_{-\infty}^{\infty} dy\, V(x-y)\, m(y)\right] \tag{1.9}$$

This can be linearized at the boundary of the paramagnetic region of the phase diagram, revealing a ferromagnetic or modulated phase according to whether the maximum of $\hat{V}(u)$ [(1.2) with $d=1$] occurs for $u=0$ or $u \neq 0$, respectively.

In this paper we complete the study by providing a trial magnetization $m(x)$ from which the wavenumber in the modulated phase is readily computed. In fact our ansatz is modeled on some exact solutions of the nonlinear integral equation (1.9) for the choice of potential (an obvious continuous generalization of the discrete ANNNI potential)

$$V(x) = \begin{cases} J_1, & |x| \leqslant \alpha \\ -J_2, & \alpha < |x| < 1 \end{cases} \tag{1.10}$$

After presenting these exact solutions and thus deducing a general trial magnetization in Section 2, we proceed in Section 3 to consider the general properties of the latter. In particular, we consider the paramagnetic–modulated and ferromagnetic–modulated phase boundaries, and the low-temperature limit. In Section 4 the particular potential (1.10) is reconsidered, and it is shown that in the low-temperature limit the variational equations are quadratic, and thus can be solved analytically. We then present the results of a numerical study of the variational equations in the purely antiferromagnetic case [$\alpha = 0$ in (1.10)], thus obtaining explicitly the variation of the wavenumber from the Lifschitz point to the ground state. In conclusion, the modulated regime of this continuous mean-field theory is contrasted to that of the discrete mean-field theory of the ANNNI model.

2. THE TRIAL MAGNETIZATION

A frequently used practical technique for obtaining good approximations to functionals of the form (1.4) is the trial function method. The task is to guess a function, with several unspecified parameters, that has the essential properties of what is expected of the maximal variational function. Then the functional is maximized with respect to the unspecified parameters.

To carry out this program in the present case, we begin by presenting some particular exact solutions of the stationary condition (1.9). These solutions immediately suggest a useful trial magnetization in general.

2.1. Some Exact Solutions of a Nonlinear Integral Equation

Consider Eq. (1.9) with the potential (1.10). Define the dimensionless temperature

$$\beta^* \equiv \beta J_1 \tag{2.1}$$

and the parameter

$$\kappa \equiv J_2/J_1 \tag{2.2}$$

which controls the degree of competition between the ferromagnetic and antiferromagnetic couplings. Then, after differentiation, (1.9) becomes

$$dm/dx = \beta^*[1 - m^2(x)]\{(1+\kappa)[m(x+\alpha) - m(x-\alpha)] - \kappa[m(x+1) - m(x-1)]\} \tag{2.3}$$

Our exact solutions can be divided into three types:

(i) Solutions of the form

$$m(x) = k\,\mathrm{sn}(4K\alpha p)\,\mathrm{sn}(4Kpx + \phi), \qquad p = [2(1-\alpha)]^{-1} \tag{2.4}$$

where sn is a Jacobian elliptic function,[6] with k the modulus and $K = K(k)$ the complete elliptic integral of the first kind. Using the addition formula

$$\operatorname{sn}(z+a) - \operatorname{sn}(z-a) = \frac{2 \operatorname{cn} z \operatorname{dn} z \operatorname{sn} a}{1 - k^2 \operatorname{sn}^2 z \operatorname{sn}^2 a} \tag{2.5}$$

with $z = px + \phi$ and $a = \alpha$, 1; noting for the choice of p in (2.4) that

$$\operatorname{sn}(4Kp) = -\operatorname{sn}(4K\alpha p) \tag{2.6}$$

and using the formula for the derivative

$$\frac{d}{dz} \operatorname{sn} z = \operatorname{cn} z \operatorname{dn} z \tag{2.7}$$

we see that (2.3) is satisfied identically when

$$2Kp = \beta^*(1 + 2\kappa) \operatorname{sn}(4K\alpha p) \tag{2.8}$$

(ii) Solutions of the form

$$m(x) = k \operatorname{sn}(4K\alpha p) \operatorname{sn}(4Kpx + \phi), \qquad p = 1/2 \tag{2.9}$$

In this case $m(x) = m(x+2)$, so the second difference in (2.3) vanishes. Use of (2.5) and (2.6) shows that we require the auxiliary condition

$$2Kp = \beta^*(1 + \kappa) \operatorname{sn}(4K\alpha p) \tag{2.10}$$

(iii) Solutions of the form

$$m(x) = k \operatorname{sn} 4Kp \operatorname{sn}(4Kpx + \phi), \qquad \alpha = 0 \tag{2.11}$$

This corresponds to the purely antiferromagnetic case. Clearly, J_1 is an irrelevant variable, and we take the dimensionless temperature as

$$\beta^* = \beta J_2 \tag{2.12}$$

The first difference in (2.3) vanishes. Again, use of (2.5) and (2.6) shows that we require an auxiliary condition

$$2Kp = -\beta^* \operatorname{sn} p \tag{2.13}$$

Hence, each of (2.4), (2.9), and (2.11) satisfies (2.3) or equivalently (1.9) (the latter, with possibly an additive constant on the right-hand side). In fact, (1.9) is satisfied exactly, since at $x = -\phi/(4Kp)$ it is simple to show that both sides of (1.9) vanish for the solutions (2.4), (2.9), and (2.11), so the additive constant is zero.

2.2. A General Ansatz

The analytic form of the above exact solutions strongly suggest a trial magnetization in general of the form

$$m(x) = c\,\mathrm{sn}(4Kpx + \phi) \tag{2.14}$$

where c, k, and p are variational parameters and ϕ is an arbitrary phase, which we will take to be K. In practice, we will use the theta-function form of sn, so that

$$m(x) = c\left(\frac{\vartheta_3(q)\,\vartheta_2(2\pi px, q)}{\vartheta_2(q)\,\vartheta_3(2\pi px, q)}\right) \tag{2.15}$$

The variational parameter k is thus replaced by q, where in the usual notation[6]

$$q = \exp[-\pi K(k)/K(k')] \tag{2.16}$$

With the particular potential (1.10) (and α fixed), the exact solutions (i) and (ii) each hold for one value of p only. The amplitude c is given explicitly and the variational parameter q is specified in terms of β^* and κ by (2.7) or (2.9). For given κ and β^*, this solution must be substituted in (1.6) and compared with the value of (1.6) obtained from (2.14) with other values of p. This allows the optimal magnetization of the form (2.14) to be determined, and will give the wavenumber p as a function of κ and β^*. In this way we can calculate the equations of the lines $p(\kappa, \beta^*) = \text{const}$ in the (κ, β^*) plane, which correspond to the global maximum of (1.6). In Section 4 we do this explicitly for low temperatures and find that the exact solution (ii) corresponds to a global maximum of (1.6) along a certain curve in the (κ, β^*) plane, but the exact solution (i) is merely a local rather than a global maximum.

The antiferromagnetic solution is valid for continuous values of p, including those wavenumbers between that of the ground state and the Lifschitz point. Thus, it only remains to optimize (2.11) with respect to the single variational parameter p. We present the results of the numerical solution of this problem in Section 5.

3. LIMITING FORMS OF THE TRIAL MAGNETIZATION

An accurate trial magnetization must display the known behavior near the paramagnetic–modulated phase boundary[7,5] and be able to reproduce the ferromagnetic solution (see Fig. 1). Here we show that the first of these features is contained in (2.15) in the limit $q \to 0$. For the latter property the

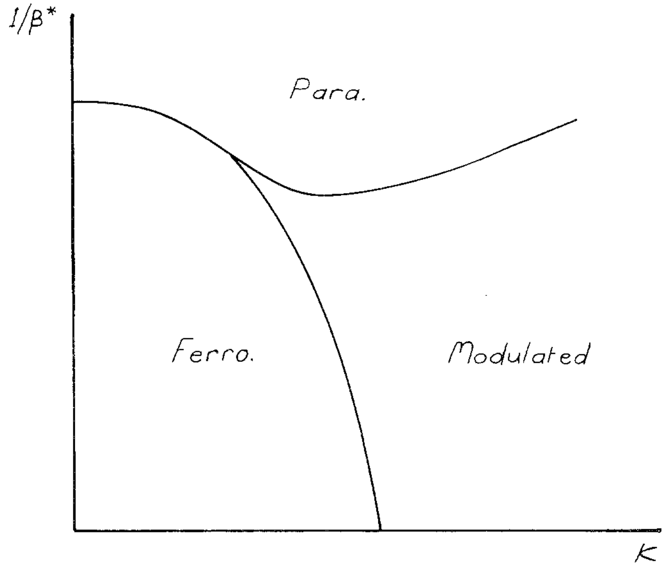

Fig. 1. A schematic diagram indicating the three phases typical of mean-field theory with competing interactions. As usual, $1/\beta^*$ denotes the dimensionless temperature and κ is a measure of the degree of competition between ferromagnetic and antiferromagnetic interactions within the system.

relevant variable is $\log(1/q)$, or, as is conventional, ε, where $q = e^{-\pi\varepsilon}$. We show that the ferromagnetic solution is reclaimed from (2.15) in the limit $\varepsilon \to 0$, $p \to 0$, $p/\varepsilon \to \text{const}$. The low-temperature limit is then studied, and again $\log(1/q)$ is the relevant variable, with the limit corresponding to $\varepsilon \to 0$.

It is interesting to note that these three limiting forms are of prominence in the theory of exactly solvable two-dimensional lattice models.[8] There the Boltzmann weights on a solvable manifold are parametrized in terms of theta functions. The limits then correspond to approaching a multicritical point, the boundary between regimes II and III (in the notation of ref. 8) and the ground state, respectively.

3.1. Paramagnetic–Modulated Phase Boundary

We know[7,5] that the critical temperature defining the paramagnetic–modulated phase boundary is given by

$$\beta_c = 1/\hat{K}(p^*) \tag{3.1}$$

where $p^* \neq 0$ maximizes $\hat{V}$. Furthermore, for a given p, the stationarity condition (1.9) permits a unique solution of the form

$$m(x) = \sum_{n=0}^{\infty} a_n(p, \beta) \cos[(4n+2)\pi p x] \tag{3.2a}$$

where

$$a_n(p, \beta) = \sum_{l=n}^{\infty} \alpha_n^l(p)[\beta \hat{V}(p) - 1]^{(2l+1)/2} \tag{3.2b}$$

To order $(\beta/\beta_c - 1)^{3/2}$, (3.2) maximizes (1.6) when[7]

$$p = p^*; \qquad \alpha_0^0 = 2, \qquad \alpha_1^1 = 2/\{3[\beta \hat{V}(3p) - 1]\}; \qquad \alpha_0^1 = -2 - \frac{1}{2}\alpha_1^1 \tag{3.3}$$

To show that the ansatz (2.15) reproduces (3.2), write

$$m(x) \sim c[m_0(q) \cos 2\pi p x + m_1(q) \cos 6\pi p x + m_2(q) \cos 10\pi p x + \cdots] \tag{3.4}$$

It is simple to check (self-consistently) that to order $(\beta/\beta_c - 1)^{3/2}$, (1.6) only involves $cm_0(q)$, $cm_1(q)$, and p. Since they are three independent variables, and our variational approximation has an expansion of the form (3.4) with three independent variables, to this order we reproduce the general expansion.

3.2. Ferromagnetic–Modulated Phase Boundary

With the ansatz (2.15), it may seem that there is no special limit at the ferromagnetic–modulated phase boundary—one merely takes $p = 0$. However, the exact solution in the antiferromagnetic regime (2.11) must contain the ferromagnetic solution when J_2 is negative. If we simply choose $p = 0$, this would imply $m(x) = 0$.

As noted in the introduction to this section, with $q = e^{-\pi\varepsilon}$, the correct limiting form is in fact $\varepsilon \to 0$, $p \to 0$, $p/\varepsilon \to s$ (constant). By the conjugate modulus transformations[6]

$$\frac{\vartheta_1(z, e^{-\pi\varepsilon})}{\vartheta_4(z, e^{-\pi\varepsilon})} = \frac{-i\vartheta_1(zi/\varepsilon, e^{-\pi/\varepsilon})}{\vartheta_2(zi/\varepsilon, e^{-\pi/\varepsilon})}, \qquad \frac{\vartheta_2(z, e^{-\pi\varepsilon})}{\vartheta_3(z, e^{-\pi\varepsilon})} = \frac{\vartheta_4(zi/\varepsilon, e^{-\pi/\varepsilon})}{\vartheta_3(zi/\varepsilon, e^{-\pi/\varepsilon})} \tag{3.5}$$

we then have

$$m(x) \sim c[1 + O(e^{-\pi/\varepsilon})] \tag{3.6}$$

and in the antiferromagnetic case (2.11)

$$m(x) \sim \tanh \pi s \tag{3.7}$$

3.3. Low-Temperature Limit

In the low-temperature limit we must have $|m(x)| \sim 1$. With the trial magnetization (2.14), this situation is realized in the limit $\varepsilon \to 0$, where use of (3.5) shows

$$m(x) \sim c \frac{\cos 2\pi xp}{|\cos 2\pi xp|} \tag{3.8}$$

In order to perform calculations, we seek a tractable form of the functional (1.6). Consider first $E_1\{m(x)\}$ as defined by (1.7). Since $m(x)$ is a periodic function of period $1/p$, we can write

$$m(x) = \sum_{n=-\infty}^{\infty} c_n e^{2\pi inpx} \tag{3.9}$$

where the c_n are the Fourier coefficients. Substituting this form in (1.7) and changing the order of the limiting procedures, we have

$$E_1 = \frac{\beta}{2} \sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} c_m c_n^* \lim_{M\to\infty} \frac{1}{2M} I_{m,n}(x; M) \tag{3.10}$$

where

$$I_{m,n}(x; M) = \int_{-M}^{M} \int_{-M}^{M} dx\, dy\, V(|x-y|)\, e^{2\pi ip(mx-ny)} \tag{3.11}$$

Now, in (3.11), change variables $x-y=\eta$, $x+y=\xi$, replace η by $-\eta$ for η negative, and ξ by $-\xi$ for ξ negative, and then replace ξ by $2M-\xi$, to show that

$$I_{m,n}(x; M) = 2\int_0^{2M} d\xi \cos \pi p\xi(m-n) \int_0^{\xi} d\eta\, V(|\eta|) \cos \pi p\eta(m+n) \tag{3.12}$$

If $m=n$, integration by parts gives

$$I_{n,n}(x; M) = 4M \int_0^{2M} d\eta\, V(|\eta|) \cos 2\pi p\eta n - 2\int_0^{2M} d\xi [\xi V(|\xi|) \cos 2\pi p\xi n] \tag{3.13}$$

while for $m \neq n$, again using integration by parts gives

$$I_{m,n}(x; M) = -\frac{2}{\pi p(m-n)} \int_0^{2M} d\xi \sin \pi p\xi(m-n) \cos \pi p\xi(m+n)\, V(|\xi|) \tag{3.14}$$

The first term in (3.13) is $O(M)$, while the second term is $O(1)$. Also, (3.14) is $O(1)$, so the only term remaining after the $M \to \infty$ limit in (3.10) is the first term of (3.13). Thus[3]

$$E_1 = \frac{\beta}{2} \sum_{n=-\infty}^{\infty} |c_n|^2 \hat{V}(pn) \tag{3.15}$$

For the choice of magnetization (2.14), using the Fourier expansion of sn,[(6)] we have

$$m(x) = \frac{2\pi c}{Kk} \sum_{n=0}^{\infty} \frac{(-1)^n q^{n+1/2} \cos(4n+2)\pi xp}{1-q^{2n+1}} \tag{3.16}$$

Hence, from (3.9), (3.15), and (3.16) we obtain

$$E_1 = \frac{\beta}{2} \left(\frac{\pi c}{Kk}\right)^2 \sum_{l=-\infty}^{\infty} \frac{\hat{V}(p(2l+1))}{(q^{-(l+1/2)} - q^{(l+1/2)})^2} \tag{3.17}$$

In the low-temperature limit

$$Kk \sim \pi/2\varepsilon + O(e^{-\pi/\varepsilon}) \tag{3.18}$$

so up to terms $O(e^{-\pi/\varepsilon})$ (assuming corrections to $1-c$ are also of this order), as $\varepsilon \to 0$,

$$E_1 \sim \frac{\beta}{2} \varepsilon^2 \sum_{l=-\infty}^{\infty} \frac{\hat{V}(p(2l+1))}{\sinh^2 \pi\varepsilon(l+1/2)} \tag{3.19}$$

Next consider the functional (1.8). For any even, antiperiodic function $m(x)$ of antiperiod $1/2p$,

$$E_2 = -\int_0^1 dx \left[\frac{1+m(x/4p)}{2} \log\left(\frac{1+m(x/4p)}{2}\right) + \frac{1-m(x/4p)}{2} \log\left(\frac{1-m(x/4p)}{2}\right)\right] \tag{3.20}$$

From (2.15) and (3.5), for $0 \leqslant x \leqslant 1/2p$,

$$m(x) \sim \left(\frac{1-e^{-\pi/\varepsilon + 4\pi xp/\varepsilon}}{1+e^{-\pi/\varepsilon + 4\pi xp/\varepsilon}}\right) + o(e^{-\pi/\varepsilon}) \tag{3.21}$$

[3] We thank the referee for pointing out this general formula and sketching its derivation.

Substituting (3.21) in (3.20), changing variables $x \to (1-\varepsilon x/\pi)$, and noting that

$$\int_0^\infty dx \log(1+e^{-x}) = \sum_{n=1}^{\infty} \frac{(-1)^{n+1}}{n^2} = \frac{\pi^2}{12} \tag{3.22}$$

gives the expansion, as $\varepsilon \to 0$,

$$E_2 \sim \pi\varepsilon/6 + O(e^{-\pi/\varepsilon}) \tag{3.23}$$

Hence, with $m(x)$ given by (2.15), up to terms of order $e^{-\pi/\varepsilon}$,

$$-\beta\psi \underset{\varepsilon \to 0}{\sim} \frac{\beta}{2}\varepsilon^2 \sum_{l=-\infty}^{\infty} \frac{\hat{V}(p(2l+1))}{\sinh^2 \pi\varepsilon(l+1/2)} + \frac{\pi\varepsilon}{6} \tag{3.24}$$

4. THE WAVENUMBER IN THE LOW-TEMPERATURE REGIME: A QUADRATIC THEORY

From Section 3.1 the wavenumber near the paramagnetic–modulated phase boundary is given by p^*, where $p^* \neq 0$ maximizes $\hat{V}(p)$.

We can calculate p in the low-temperature regime from (3.24). Here we do this for the choice of potential (1.10).

4.1. A Conjugate Modulus-Type Transformation

With the potential (1.10),

$$\beta\hat{V}(p) = \frac{\beta^*}{\pi p}\left[(1+\kappa)\sin 2\pi\alpha p - \kappa \sin 2\pi p\right] \tag{4.1}$$

Thus, from (3.24) we see that it is necessary to obtain a small-ε expansion of series of the form

$$S(x) = \sum_{k=-\infty}^{\infty} \frac{\sin 2\pi x(k+1/2)}{(k+1/2)\sinh^2 \pi\varepsilon(k+1/2)} \tag{4.2}$$

To do this, we first derive the conjugate modulus-type transformation

$$S(x) = \pi\left(\frac{1}{2\varepsilon^2} - \frac{2(x-1/2)^2}{\varepsilon^2} - \frac{1}{3}\right) + \frac{2(x-1/2)}{\varepsilon} \sum_{k=-\infty}^{\infty}{}' \frac{e^{-2\pi k(x-1/2)/\varepsilon}}{k\cosh \pi k/\varepsilon}$$
$$+ \frac{1}{\pi} \sum_{k=-\infty}^{\infty}{}' \frac{e^{-2\pi k(x-1/2)/\varepsilon}}{k^2 \cosh \pi k/\varepsilon} + \frac{1}{\varepsilon} \sum_{k=-\infty}^{\infty}{}' \frac{e^{-2\pi k(x-1/2)/\varepsilon} \sinh \pi k/\varepsilon}{k\cosh^2 \pi k/\varepsilon} \tag{4.3}$$

where the primes on the summation denote that the $k=0$ term is to be omitted. The transformation is valid for $0 < x < 1$.

Consider the contour integral

$$\int_{C_N} \frac{dz\, e^{2\pi i(x-1/2)z}}{z \cos \pi z \sinh^2 \pi \varepsilon z} \tag{4.4}$$

where the contour C_N is a circle of radius N centered on the origin. In the limit $N \to \infty$, for $|x-1/2|<1$, this integral is zero. Therefore, the sum of residues must be zero. The original series (4.2) results from evaluating the residues at $z=k+1/2$, while the transformed series (4.3) come from the remaining double poles at $z=ni/\varepsilon$ $(n \neq 0)$ and the third-order pole at $z=0$.

For $0<x<1$ the asymptotic behavior is thus

$$S(x) \underset{\varepsilon \to 0}{\sim} \pi\left(\frac{1}{2\varepsilon^2}-\frac{2(x-1/2)^2}{\varepsilon^2}-\frac{1}{3}\right)+O[\max(e^{-\pi/\varepsilon}, e^{-2\pi x/\varepsilon}, e^{-2\pi(1-x)/\varepsilon})] \tag{4.5}$$

When $x=1-v$, $v/\varepsilon \to 0$, further terms in (4.3) contribute. In this limit the three infinite series in (4.3) behave, up to corrections $O(e^{-\pi/\varepsilon})$, as

$$2\log(1-e^{-4\pi v/\varepsilon}), \quad \frac{\pi^2}{6}+\frac{4\pi v}{\varepsilon}\log(1-e^{-4\pi v/\varepsilon}), \quad -2\log(1-e^{-4\pi v/\varepsilon}) \tag{4.6}$$

respectively. Therefore

$$S(x) \sim \pi\left(\frac{1}{2\varepsilon^2}-\frac{2(x-1/2)^2}{\varepsilon^2}\right) \tag{4.7}$$

Also of interest is the case $1<x<2$. From (4.3)

$$S(x) = -S(x-1) \tag{4.8}$$

Since $|x-1|<1$, we can use (4.3) to conclude

$$S(x) \sim -\pi\left(\frac{1}{2\varepsilon^2}-\frac{2(x-3/2)^2}{\varepsilon^2}-\frac{1}{3}\right) \tag{4.9}$$

4.2. Quadratic Expressions for the Free Energy

In each of the cases (i) $0<p<1/2$, (ii) $p=1/2-v$, $v/\varepsilon \to 0$, and (iii) $1/2<p<1$ the free energy is quadratic in the two variational parameters p and ε [by the periodicity of $p\hat{V}(p)$ we can assume $p<1$]. From (3.24), (4.1), (4.5), (4.7), and (4.9) we have for (i) and (ii)

$$-\beta\psi = \beta^*\left(-\frac{\varepsilon^2\chi}{12p}+\frac{\pi\varepsilon}{6(\beta^*)^2}+E_0(p, \kappa, \alpha)\right) \tag{4.10}$$

where $\chi = 1,\ 1+\kappa$ for cases (i) and (ii), respectively, and

$$E_0(p, \kappa, \alpha) = p[2\kappa - 2\alpha^2(1+\kappa)] + (-\kappa + \alpha + \kappa\alpha) \qquad (4.11)$$

while for (iii), assuming further that $p\alpha < 1/2$,

$$-\beta\psi = \beta^* \left(-\frac{\varepsilon^2(1+2\kappa)}{12p} + \frac{\pi\varepsilon}{6(\beta^*)^2} + E_0(p, \kappa, \alpha) \right) \qquad (4.12)$$

where

$$E_0(p, \kappa, \alpha) = (1+\kappa)(-2\alpha^2 p + \alpha) + \kappa(-2p + 3 - 1/p) \qquad (4.13)$$

Maximizing with respect to ε gives for (i) and (ii)

$$\varepsilon = \pi p/(\beta^* \chi) \qquad (4.14)$$

$$-\beta\psi = \beta^* \{\pi^2 p/[12(\beta^*)^2 \chi] + E_0(p, \kappa, \alpha)\} \qquad (4.15)$$

while for (iii)

$$\begin{aligned} \varepsilon &= \pi p/[\beta^*(1+2\kappa)] \\ -\beta\psi &= \beta^* \{\pi^2 p/[12(\beta^*)^2(1+2\kappa)] + E_0(p, \kappa, \alpha)\} \end{aligned} \qquad (4.16)$$

4.3. The Ground States

For given α and κ we will first consider the maximization of the negative of the ground state-energy E_0 with respect to p. From (4.11) and (4.13), the following results are evident.

Suppose

$$\kappa < \alpha^2/(1-\alpha^2) \qquad (4.17)$$

Then we have the ferromagnetic ground state $p = 0$. If

$$\kappa = \alpha^2/(1-\alpha^2) \qquad (4.18)$$

then all wavenumbers $0 \leqslant p \leqslant 1/2$ correspond to the ground state. If

$$\kappa > \alpha^2/(1-\alpha^2) \qquad (4.19)$$

then the ground-state wavenumber is

$$p = [2 + 2\alpha^2(1+\kappa)/\kappa]^{-1/2} \qquad (4.20)$$

[note that this is consistent with the condition $\alpha p < 1/2$ used in the derivation of (4.12)].

Thus, the largest wavenumber occurs when $\kappa \to \infty$ and

$$p = (2 + 2\alpha^2)^{-1/2} \tag{4.21}$$

In particular, for all κ and α

$$p < [2(1-\alpha)]^{-1} \tag{4.22}$$

and so the exact solution (2.4), which has wavenumber $[2(1-\alpha)]^{-1}$, does not maximize the functional (1.6) in the low-temperature limit. On the other hand, for all α, the exact solution (2.9), which has wavenumber 1/2, corresponds to a minimum of the ground-state energy.

4.4. Variation of the Wavenumber with Temperature

Consider now the quadratic low-temperature expansions (4.15) and (4.16). We first determine the destabilization of the ferromagnetic phase in the (κ, β^*) plane. From (4.15) this occurs when

$$\kappa > \frac{\alpha^2}{1-\alpha^2} - \frac{\pi^2}{24(\beta^*)^2(1-\alpha^2)} \tag{4.23}$$

In fact, since (4.15) is linear in p, the maximal wavenumber is $p \sim 1/2$ [for (4.16) to be valid we require $1/2 - p > O(1/\beta^*)$]. Thus, to order $\exp(-2\alpha\beta^*)$, which is the lowest order correction ignored in (4.15), the wavenumber is discontinuous across the ferromagnetic–modulated phase boundary. If such corrections were included in the free energy, we would expect the degeneracy to be removed, but the width of the variation from $p = 0$ to $\sim 1/2$ to be exponentially small.

A bound on the boundary of the region for which $p < 1/2$ can be calculated from (4.15) with $\chi = 1 + \kappa$. We have $p < 1/2$ as the maximal wavenumber when, to order $1/(\beta^*)^2$,

$$\kappa \leqslant \frac{\alpha^2}{1-\alpha^2} - \frac{\pi^2}{24(\beta^*)^2} \tag{4.24}$$

To complete the phase diagram in the low-temperature regime, consider the region

$$\kappa > \frac{\alpha^2}{1-\alpha^2} - \frac{\pi^2}{24(\beta^*)^2} \tag{4.25}$$

Then from (4.16) the maximal wavenumber is

$$p = \kappa^{1/2}\left(2\kappa + 2\alpha^2(1+\kappa) - \frac{\pi^2}{12(\beta^*)^2(1+2\kappa)}\right)^{-1/2} \tag{4.26}$$

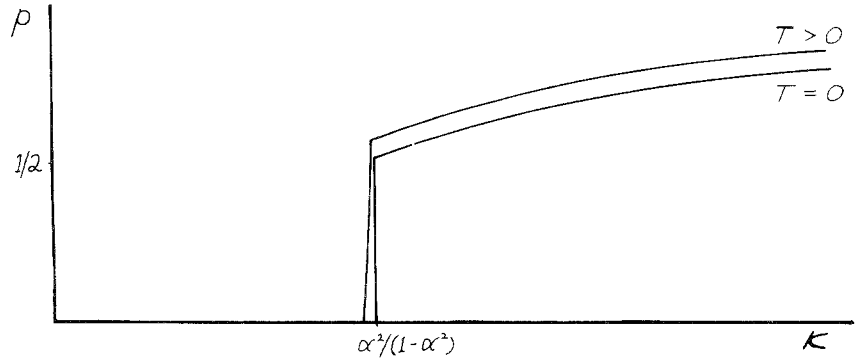

Fig. 2. A schematic diagram showing the wavenumber as a function of κ for the potential (1.10) at zero and nonzero temperature.

Thus, the lines of constant p in the (κ, β^*) plane, for $p > 1/2$, are given by

$$\kappa = \frac{2\alpha^2 p^2}{2(\alpha^2+1)\,p^2-1} - \frac{\pi^2}{24(\beta^*)^2} + O\left(\frac{1}{(\beta^*)^4}\right) \tag{4.27}$$

A schematic summary of these results is given in Fig. 2.

5. THE MODULATED REGIME FOR THE PURELY ANTIFERROMAGNETIC INTERACTION

When $\alpha = 0$ in (1.10) we have the purely antiferromagnetic interaction

$$V(x) = \begin{cases} -J_2, & |x| \leqslant 1 \\ 0, & |x| > 1 \end{cases} \tag{5.1}$$

From Section 2.1, with the dimensionless temperature defined by (2.12), the trial magnetization

$$m(x) = \frac{\vartheta_1(2\pi p, q)\,\vartheta_2(2\pi p x, q)}{\vartheta_4(2\pi p, q)\,\vartheta_3(2\pi p x, q)} \tag{5.2}$$

with q specified by

$$\pi p = -\frac{\beta^* \vartheta_1(2\pi p, q)}{\vartheta_2(q)\,\vartheta_3(q)\,\vartheta_4(2\pi p, q)} \tag{5.3}$$

satisfies the stationarity condition (1.9) exactly. Thus, the only independent variational parameter is p.

The wavenumber at the Lifschitz point is given by the first maximum of

$$\beta\hat{V}(p) = -\beta^*(\sin 2\pi p)/\pi p \tag{5.4}$$

which occurs when

$$p \equiv p^* \simeq 0.7152 \tag{5.5}$$

and the critical temperature is

$$1/\beta_c^* = -(\sin 2\pi p^*)/\pi p^* \simeq 0.4344 \tag{5.6}$$

In the low-temperature region, minor modification to the working in Section 4 shows that, to order

$$e^{-\pi/\varepsilon} \quad \text{with} \quad \varepsilon = \pi p/\beta^* \tag{5.7}$$

the maximal wavenumber is

$$p = [2 - (\pi^2/24\beta^{*2})]^{-1/2} \tag{5.8}$$

In particular, at zero temperature

$$p = 1/\sqrt{2} \simeq 0.7071 \tag{5.9}$$

Thus, as the temperature is increased from zero to the critical value (5.6), the wavenumber increases from 0.7071 to 0.7152, a change in the second decimal place only.

To calculate the variation of the wavenumber as a function of temperature numerically, we make use of the analytic result (5.8). From (5.7) we would expect (5.8) to be accurate to three decimal places (at least) for temperatures less than $1/\beta^* = 1/10$, since corrections to the free energy are of order 10^{-7} or less. As $1/\beta^*$ is increased, the trial value of p is obtained from quadratic extrapolation, and the value of q calculated from (5.3)

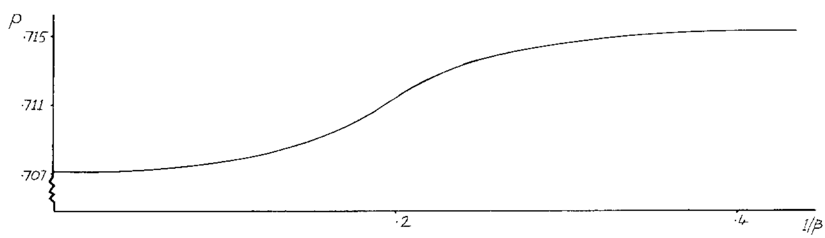

Fig. 3. A plot of the wavenumber as a function of the dimensionless temperature $1/\beta^*$ for the purely antiferromagnetic potential (5.1).

using the Newton–Raphson formula. Since $q < \exp(-\pi\sqrt{2}/10) \simeq 0.64$, accurate approximations to the theta functions can be obtained by including only the first few terms of the series expansion. The value of the functional (1.6) is then calculated, and the procedure repeated with $1/\beta^*$ fixed but other values of p until the maximal value is found. The results of the calculation are displayed in Fig. 3.

6. CONCLUSION AND CONTRAST WITH THE ANNNI MODEL

As a trial magnetization to well describe the modulated regime of the exact mean-field theory of competing interactions, we have proposed an elliptic function ansatz (2.14) with the amplitude, modulus, and period as variational parameters. For a particular choice of potential (1.10), which is an obvious continuous version of the ANNNI model between plane interaction, we have studied the equations analytically in the low-temperature regime.

At zero temperature, there is a particular choice of interaction parameters (4.18) for which all wavenumbers from 0 to 1/2 correspond to the ground state. As the strength of the competition is increased above this value, the ground-state wavenumber varies smoothly with the interaction parameters. At nonzero temperature the degeneracy is removed, and the wavenumber is a smooth function of the interaction parameters.

The ground state of the ANNNI model also has a multiphase point ($\kappa = 1/2$) at which a countably infinite sequence of phases coexist.[4] However, for $\kappa > 1/2$ the ground state sticks to the $\langle 2 \rangle$phase. At low temperature the $\langle 2 \rangle$phase remains stable, but the multiphase point gives rise to a complex wedge of commensurate phases.

The basic mechanism for the existence of the commensurate phases in the ANNNI model is well known: it is a coupling phenomena with the underlying lattice. In the continuous case there is no underlying lattice. Not surprisingly, then, we have provided evidence in a particular case, and would expect in general, that for nonzero temperatures the wavenumber is a smooth function of the temperature and interaction parameters.

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