Hamiltonian Studies of the Two-Dimensional Axial Next-Nearest-Neighbor Ising (ANNNI) Model. I. Perturbation Expansions

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A one-dimensional quantum Hamiltonian which is equivalent to the two-dimensional axial next-nearest-neighbor Ising (ANNNI) model is studied through the derivation and analysis of weak- and strong-coupling perturbation expansions. The phase diagram is constructed and the nature of the phase transitions discussed. In particular, we conclude (i) that there is no Lifshitz point on the ferromagnetic/paramagnetic phase boundary, (ii) there appears to be a Lifshitz point on the antiphase/paramagnetic phase, (iii) above the antiphase Lifshitz point the single transition from paramagnetism to the antiphase is probably continuous and marked by algebraic singularities, (iv) below the antiphase Lifshitz point the transition from paramagnetism to the antiphase is via two transitions, the upper of which is probably of the Kosterlitz/Thouless type, (v) the intermediate phase is presumably incommensurate although the perturbation methods do not directly probe this question.

I. INTRODUCTION

The axial next-nearest-neighbor Ising (or ANNNI) model has received considerable attention recently. Much of this interest stems from interest in systems exhibiting incommensurate/commensurate transitions (for a review see Villain[1]). The ANNNI model appears to be one of the simplest models to exhibit such transitions.

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In two dimensions, the dimensionality of interest here, the model is specified by the Hamiltonian

$$\mathcal{H} = -\sum_{(i,j)} \left(J_1 s_{i,j} s_{i+1,j} + J_2 s_{i,j} s_{i+2,j} + J_0 s_{i,j} s_{i,j+1} \right) \qquad (1.1)$$

where the sum is over the sites of a square lattice, which are populated by Ising spin variables ($s_{i,j} = \pm 1$). The nearest-neighbor interactions (J_0, J_1) are ferromagnetic, but the axial next-nearest-neighbor interaction (J_2) is taken as antiferromagnetic and hence competing. Higher-dimensional versions are defined similarly with the axial antiferromagnetic interaction restricted to one of the spatial axes of a hypercube.

The ANNNI model was originally introduced (in three dimensions) by Elliot[2]) to explain the modulated phases observed in some rare earth compounds. Interest in the model was renewed by the work of Bak and von Boehm,[3] who investigated the phase diagram within mean field theory emphasizing the role of nonlinear excitations such as solitions, and of Selke[4] and Hornreich et al.,[5] who initiated a Monte Carlo study. This was subsequently extended and refined by Selke and Fisher.[6] Other recent investigations of the two-dimensional ANNNI model are contained in Refs. 7–14. Much of this work will be discussed further below. One should also note the work of Fisher and Selke,[15] Villain and Gordon,[16] and Bak[17] which has resolved much of the low-temperature phase diagram for dimensionalities greater than two. The high-temperature behavior of the three-dimensional model has also been probed by series expansions.[18]

The aim of this series of papers is to investigate the two-dimensional ANNNI model from the point of view of its analogous quantum Hamiltonian. The equivalence of a statistical mechanical system in d spatial dimensions and a quantum field theory in $[(d-1)+1]$ space time dimensions is well known (for a recent review see Kogut[19]). In particular, the correspondence between a transfer matrix and a quantum Hamiltonian[19–21] has been extensively exploited to study, by various methods, phase transitions in spin systems.[19,21–29] These successes have established these methods as a powerful approach to the study of phase transitions in two dimensions.

In this article, we set up the quantum Hamiltonian analog of the $d = 2$ ANNNI model, which is then studied by the analysis of systematic perturbation expansions of various physical quantities. The following paper supplements these results with finite lattice calculations and their analysis via finite-size scaling. A letter reporting the Hamiltonian formulation and giving an initial summary of some of our results has already appeared.[8] The Hamiltonian formulation has also been developed by Rujan.[9] We shall discuss his results in more detail below.

This paper is arranged as follows. In the next section we derive the appropriate quantum Hamiltonian and describe a duality transformation linking the weak and strong coupling regimes. The soluble limits of the model are identified in Section 3, while Section 4 describes the derivation of systematic perturbation expansions. These are analyzed in Section 5. The paper closes with an overall summary and discussion in Section 6.

2. QUANTUM HAMILTONIAN FORMULATION OF THE ANNNI MODEL

2.1. Derivation of the Quantum Hamiltonian

Let T denote the transfer matrix of a statistical mechanical system in a direction specified by the coordinate x_d of a d-dimensional lattice. The analogous quantum Hamiltonian is then defined by[19-21]

$$T = 1 - \tau H + O(\tau^2) \tag{2.1}$$

where τ is a small (strictly infinitesimal) parameter. The free energy of the statistical mechanical system (given by the largest eigenvalue of T) is now related to the ground-state energy of H, while the correlation length is given by the reciprocal of the mass gap of H. The Hamiltonian H refers to a quantum mechanical system on a $(d-1)$-dimensional lattice with time continuous.

In almost all previous applications of this approach (see, e.g., Refs. 19, 21, 26, 29), the statistical mechanical system of interest has been spatially isotropic. In the case of the ANNNI model (1.1) this is not so. Hence two different quantum Hamiltonians can, in principle, be defined using the transfer matrices in x and y directions, respectively. Here we consider only the latter. This Hamiltonian was described by Barber and Duxbury[8]; see also Rujan,[9] who discussed its derivation in some detail. For completeness, we briefly rederive the Hamiltonian here.

Consider the row-to-row (y-direction) transfer matrix T of (1.1). Since the axial next-nearest-neighbor interaction J_2 affects only the self-energy of a row, the method of Schultz, Lieb, and Mattis[30] can be easily extended to write T in terms of Pauli spin matrices, σ_m^x, σ_m^z, defined on a one-dimensional chain. Hence, apart from a multiplicative constant, we obtain

$$T = V_1^{1/2} V_2 V_1^{1/2} \tag{2.2}$$

where

$$V_1 = \exp\left[\sum_m (K_1 \sigma_m^z \sigma_{m+1}^z + K_2 \sigma_m^z \sigma_{m+2}^z) \right] \tag{2.3}$$

and

$$V_2 = \exp\left(\sum_m K_0^* \sigma_m^x \right) \tag{2.4}$$

with $K_i = \beta J_i$, $i = 0, 1, 2$ and

$$K_0^* = -\tfrac{1}{2}\ln(\tanh K_0) \tag{2.5}$$

We now seek to write T in the form (2.1) by appropriately defining a suitable expansion parameter τ. To do so, set $\tau = K_0^*$, $K_1 = \lambda \tau$, and $K_2 = -\kappa K_1 = -\kappa \lambda \tau$, where λ and κ are to be finite. If we now take the limit

$$K_0 \to \infty, \qquad K_1, K_2 \to 0 \tag{2.6a}$$

with

$$\lambda = K_1 e^{2K_0} = O(1), \qquad \kappa = -K_2/K_1 = O(1) \tag{2.6b}$$

we can neglect the noncommutitivity of V_1 and V_2 to obtain

$$T = 1 - \tau H + O(\tau^2) \tag{2.7}$$

as $\tau = K_0^* \sim e^{-2K_0} \to 0$. The operator

$$H = -\sum_m \sigma_m^x - \lambda \sum_m (\sigma_m^z \sigma_{m+1}^z - \kappa \sigma_m^z \sigma_{m+2}^z) \tag{2.8}$$

is our required quantum Hamiltonian analog of the $d = 2$ ANNNI model (1.1), the parameter $\lambda \propto 1/T$ playing the role of temperature.

The key assumption behind the quantum Hamiltonian approach to statistical mechanical systems is that the highly anisotropic limit (2.6) does not change the universality class of the problem. This assumption appears to be borne out by the various applications of the approach to standard (and spatially isotropic) statistical mechanical models (see references cited above). While we have no evidence that the limit is not as innocuous for the ANNNI model, it is probably wise to keep this limit in mind when assessing the results of the Hamiltonian approach and comparing them to those of more conventional treatments of (1.1).

2.2. Duality

For $\kappa = 0$, (2.8) reduces to the $d = 1$ transverse Ising model, which is the quantum Hamiltonian analog of the nearest-neighbor Ising model.[21] In this case, Fradkin and Susskind[21] showed that the model was self-dual under the transformation

$$\mu_m^x = \sigma_m^z \sigma_{m+1}^z, \qquad \mu_m^z = \prod_{m' < m} \sigma_{m'}^x \tag{2.9}$$

Here the μ variables are again Pauli matrices but associated with the bonds

(sites of the dual lattice) of the chain, dual site m being on the bond connecting sites m and $m + 1$ of the original chain.

The transformation (2.9) can also be applied to (2.8) to give[8,9] *the dual Hamiltonian*

$$H_D = -\sum_m \mu_m^z \mu_{m+1}^z - \lambda \sum_m (\mu_m^x - \kappa \mu_m^x \mu_{m+1}^x) \qquad (2.10)$$

In writing this we have neglected the question of boundary conditions, which is valid in the thermodynamic limit. For finite chains some care is needed.[9,10] The Hamiltonians (2.8) and (2.10) will form the basis of the calculations reported in this series of papers.

3. EXACT RESULTS

Neither (2.8) nor (2.10) for arbitrary λ and κ appears to be analytically diagonalizable. There are, however, four limits in which the eigenvalues can be obtained exactly. Moreover, an understanding of the behavior of (2.8) and/or (2.10) in these limits facilitates the analysis of the general case by various approximations.

3.1. $\lambda = \infty$, κ Finite

We consider first the limit $\lambda \to \infty$, κ finite which corresponds to (1.1) in the limit of zero temperature. In this limit, the first term in (2.8) can be neglected and the ground state is that configuration (in a basis which diagonalizes σ_m^z at each site) which minimizes

$$E_0 = -\sum_m (\sigma_m^z \sigma_{m+1}^z - \kappa \sigma_m^z \sigma_{m+2}^z) \qquad (3.1)$$

This corresponds to the energy of one-dimensional Ising chain with ferromagnetic nearest- and antiferromagnetic next-nearest-neighbor interactions. This problem has been solved by Stephenson[31] and Hornreich et al.[5]

The nature of the ground state depends on κ. For $\kappa < 1/2$, the ground state is ferromagnetic and twofold degenerate, the states being distinguished by the *ferromagnetic order parameter*

$$\Gamma_F = \lim_{M \to \infty} \frac{1}{M} \left\langle \sum_{m=1}^{M} \sigma_m^z \right\rangle \qquad (3.2)$$

where $\langle \cdot \rangle$ denotes an expectation value with respect to the ground state wave function and M is the number of sites.

For $\kappa > \frac{1}{2}$, the ground state consists of alternate pairs of up ($\sigma_m^z = 1$) and down ($\sigma_m^z = -1$) spin. This corresponds to the (2, 2)-*antiphase* state[6]

of (1.1). A suitable order parameter is

$$\Gamma_A = \lim_{M \to \infty} \frac{\sqrt{2}}{M} \left\langle \sum_{m=1}^{M} e^{iq_m} \sigma_m^z \right\rangle \tag{3.3}$$

where $q_m = (2\pi m - 1)/4$. Note that in this case, Γ_A is complex and hence the antiphase is characterized by a two-dimensional order parameter.[11] The degeneracy of the ground state itself is four.

At $\kappa = \frac{1}{2}$, the ground state is highly degenerate. Inspection of (3.1) shows that if we start with one of the ferromagnetic ground states we may reverse without cost in energy any number of spins as long as we break twice as many next-nearest-neighbor bonds as nearest-neighbor bonds. Thus the ground states consist of any arbitrary sequence of alternatively "up" and "down" domains, the domains consisting of at least two spins. For a chain of M sites with free ends, Redner[32] has shown that the number of such states is $2F_{M+1}$, where F_k is the kth Fibonacci number generated by

$$F_{k+2} = F_{k+1} + F_k, \qquad F_1 = F_2 = 1 \tag{3.4}$$

For periodic boundary conditions, which will be of more interest to us, we show in Appendix A that the degeneracy of a chain of $M = 4t$ sites is

$$\Omega(t) = 2 + 8t \sum_{\nu=1}^{t} \frac{(4t - 2\nu - 1)!}{(2\nu)! (4t - 4\nu)!} \tag{3.5}$$

We note that in the limit $M \to \infty$, the residual entropy per site,

$$S = \lim_{t \to \infty} \frac{1}{4t} \ln \Omega(t) = \ln\left[(1 + \sqrt{5})/2 \right] \tag{3.6}$$

which agrees, as expected, with Redner's result and also with that found from the exact expression[5,31] of the free energy of (3.1) in the limit $T \to 0$ and $k = 1/2$.

3.2. $\lambda = 0$, κ Finite

The other trivial limit of (2.8) is $\lambda \to 0$, corresponding to the high-temperature limit of (1.1). Here the ground state of (2.8) is nondegenerate; the ground-state wave function Φ_0 being such that $\sigma_m^x \Phi_0 = \Phi_0$ for all m. Alternatively, this state can be described as the ferromagnetically ordered ground state of the dual Hamiltonian (2.10). This leads us to introduce the dual-order parameter

$$\Gamma_D = \lim_{M \to \infty} \frac{1}{M} \sum_m \langle \mu_m^z \rangle \tag{3.7}$$