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LETTER TO THE EDITOR

A quantum Hamiltonian approach to the two-dimensional axial next-nearest-neighbour Ising model

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Abstract. A quantum Hamiltonian analogue of the two-dimensional axial next-nearest-neighbour Ising (ANNNI) model is presented. The phase diagram is investigated by the analysis of perturbation series and by finite-lattice methods.

Systems exhibiting spatially modulated phases are currently of considerable interest. (For a recent review see Villain (1980)). The simplest non-trivial model to exhibit such phases is the so-called ANNNI or axial next-nearest-neighbour Ising model (Hornreich *et al* 1978, Selke and Fisher 1980, Villain and Bak 1981, and references cited in these papers). In two dimensions, this model is specified by the Hamiltonian

$$\mathscr{H} = -\sum_{(i,j)} (J_1 S_{i,j} S_{i+1,j} - J_2 S_{i,j} S_{i+2,j} + J_0 S_{i,j} S_{i,j+1}), \tag{1}$$

where the spins S_{ij} $(= \pm 1)$ populate the sites of a square lattice. All coupling constants J_i, $i = 0, 1, 2$, are positive so that the nearest-neighbour interactions are ferromagnetic but the axial next-nearest-neighbour interaction in the x direction is antiferromagnetic.

In this Letter, we summarise a detailed investigation of the phase diagram of the ANNNI model based on the associated quantum Hamiltonian field theory†. Specifically, we have considered the $(1+1)$-dimensional quantum Hamiltonian

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

Here the index m labels the sites of a linear chain and the σ_m are Pauli spin matrices. Following Fradkin and Susskind (1978), (2) can be related to the transfer matrix of (1) in the y direction in the limit $J_0 \to \infty$, $J_1, J_2 \to 0$ with

$$\lambda = \beta J_1 \exp(2\beta J_0), \qquad \lambda' = \beta J_2 \exp(2\beta J_0), \tag{3}$$

finite. The ground state energy of (2) corresponds to the free energy of (1) (see e.g. Kogut 1979). The natural parameters in which to discuss the ground state properties are λ (corresponding to the temperature: $\lambda \propto 1/T$) and the ratio $\kappa = \lambda'/\lambda = J_2/J_1$.

The ground state of (2) can be determined analytically in four limits.

† This limit has also been considered recently by Rujan (1981), who however did not develop systematic perturbation expansions.

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(i) $\lambda \to \infty$ (*i.e.* $T \to 0$), κ *fixed*
In this limit, we may choose a basis in which all σ_m^z are diagonal. For $0 \leqslant \kappa < \frac{1}{2}$, the ground state is doubly degenerate, the two states being distinguished by the order parameter $\Gamma_F = \langle \sigma_m^z \rangle$. For $\kappa > \frac{1}{2}$, the ground state is fourfold degenerate and consists of alternating pairs of up ($\sigma_m^z = +1$) and down ($\sigma_m^z = -1$) spins. An appropriate order parameter is $\Gamma_A = \frac{1}{4}\langle \sigma_m^z + \sigma_{m+1}^z - \sigma_{m+2}^z - \sigma_{m+3}^z \rangle$. This phase corresponds to the $(2-2)$ anti-phase of (1). For $\kappa = \frac{1}{2}$, the ground state is highly degenerate: any spin configuration is a ground state provided that either $\sigma_m^z = \sigma_{m+1}^z$ or $\sigma_m^z = \sigma_{m-1}^z$ for all m.

(ii) $\lambda = \lambda' = 0$ (*i.e.* $T \to \infty$)
In this case the ground state is non-degenerate and such that $\sigma_m^x = 1$, all m. Alternatively, the state can be characterised as the ferromagnetically *ordered* state of the dual Hamiltonian

$$H_D = -\sum_m [\mu_m^z \mu_{m+1}^z + \lambda(\mu_m^x - \kappa \mu_m^x \mu_{m+1}^x)], \tag{4}$$

which follows from (2) by the dual transform (Fradkin and Susskind 1978)

$$\mu_m^x = \sigma_m^z \sigma_{m+1}^z, \qquad \mu_m^z = \prod_{m'<m} \sigma_{m'}^x, \tag{5}$$

where the dual spins are defined on the *bonds* of the original chain. The order parameter $\Gamma_D = \langle \mu_m^z \rangle$ of (4) is then a *disorder parameter* characterising the disordered (high-temperature) phase of (2).

The other soluble limits of (2) are less trivial and exhibit phase transitions. They are as follows.

(iii) $\kappa = 0$, $0 \leqslant \lambda \leqslant \infty$
In this case both (2) and (4) reduce to the transverse Ising model.

(iv) $\kappa \to \infty$, $\lambda \to \infty$, $\lambda\kappa = \lambda'$ *finite*
Here (2) decouples into two transverse Ising models and (4) reduces to the XY chain. Thus from known results (Pfeuty 1970, McCoy 1968)

$$\Gamma_F(\lambda, \lambda' = 0) = (1 - 1/\lambda^2)^{1/8}, \qquad \Gamma_D(\lambda, \lambda' = 0) = (1 - \lambda^2)^{1/8}, \tag{6}$$

and

$$\Gamma_A(\lambda = 0, \lambda') = (1 - 1/\lambda'^2)^{1/8}, \qquad \Gamma_D(\lambda = 0, \lambda') = (1 - \lambda'^2)^{1/4}, \tag{7}$$

which identify the points $\lambda = 1$, $\lambda' = 0$ and $\lambda = 0$, $\lambda' = 1$ as conventional critical points.

To explore the phase diagram away from these soluble points, we have generated Raleigh–Schrödinger perturbation expansions (Hamer *et al* 1979, Kogut 1979) about the trivial limits (i) and (ii). The actual series generated were the following.

(a) *Weak-coupling*, $0 \leqslant \kappa < \frac{1}{2}$: ground state energy to order 12 in $1/\lambda^2$, ferromagnetic order parameter Γ_F to order 12 in $1/\lambda^2$, and kink mass (weak-coupling mass gap) to order 11 in $1/\lambda$.

(b) *Weak-coupling*, $\kappa > \frac{1}{2}$: ground state energy to order 7 in $1/\lambda^2$ and anti-phase order parameter Γ_A to order 7 in $1/\lambda^2$.

(c) *Strong-coupling, all* κ: ground state energy to order 13 in λ and disorder parameter Γ_D to order 13 in λ.

These series were analysed by standard methods, with phase boundaries being located by the ratio method and the poles of appropriate Padé approximants. This diagram is depicted in figure 1.

To supplement the strong-coupling perturbation expansions, we have also carried out finite-lattice calculations for lattices up to $M = 14$ sites with periodic boundary

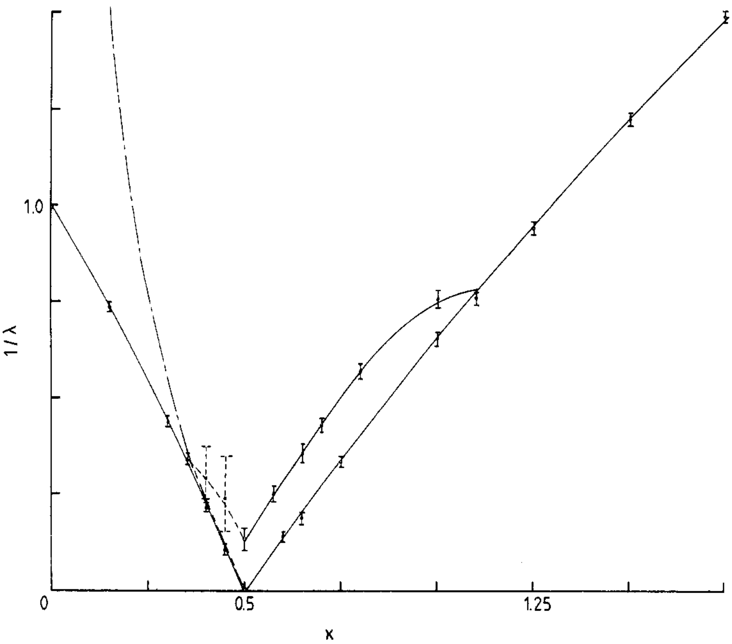

Figure 1. Phase diagram of the quantum Hamiltonian analogue of the ANNNI model. The error bars indicate the spread of the estimates from strong- and weak-coupling series expansions and finite-lattice calculations. The 'Lifshitz points' are located at $\kappa = 0.35 \pm 0.1$, $\lambda = 2.7 \pm 0.1$ and $\kappa = 1.1 \pm 0.1$, $\lambda = 1.3 \pm 0.1$. The chain curve is the special line along which Peschel has shown that the model is massive.

conditions. The strong-coupling phase boundary was then determined by finite-size scaling of the mass gap (Hamer and Barber 1980). Some care has to be taken in choosing the appropriate lattice sizes to scale, since for $\kappa > 0.35$, the first excited state no longer lies in the $k = 0$ (zero momentum) sector. As a result, we have been unable to obtain any data to apply finite-size scaling for $0.35 < \kappa < 0.5$ and only limited data for $\kappa > 0.5$. On the other hand, it is tempting to interpret the k-sector variation as heralding the eventual onset of a modulated phase. Since on a finite lattice of M sites the only possible wavevectors are integral multiples of $2\pi/M$, we do not find a continuous variation in the k sector as κ increases from 0.35. Instead, the k sector containing the first excited state jumps discontinuously, the number of jumps increasing as M increases. For $\kappa > 1.1$, the first excited state always lies in the $k = M/4$ sector, consistent with a direct transition to the anti-phase state.

Let us now summarise the actual evidence for figure 1, together with our conclusions regarding the natures of the various transitions. This is most conveniently done as a function of κ.

(i) $0 \leq \kappa < 0.35$

Here a single Ising-like transition is expected (Hornreich *et al* 1978, Selke and Fisher 1980). This expectation is confirmed: the disorder parameter, ferromagnetic order parameter and kink mass all vanishing algebraically with exponents of $\frac{1}{8}$, $\frac{1}{8}$ and 1 respectively.

(ii) $0.35 \leq \kappa < 0.5$

The weak-coupling boundary is accurately determined by the kink mass which continues to vanish *linearly* for all $0 \leq \kappa < 0.5$. On the other hand, Padé approximants to $d(\lg \Gamma_F)/d(\lambda^{-2})$, which are consistent for $\kappa < 0.35$, become very inconsistent. Padé approximants to the logarithmic derivative of $d(\lg \Gamma_F)/d(\lambda^{-2})$ are better behaved, exhibiting a pole in agreement with the kink-mass series. Taken at face value, this implies that $\Gamma_F \sim \exp\{-a/[1-\lambda_c^2(\kappa)/\lambda^2]^\sigma\}$ with $\sigma \sim 0.5$–1.0. In the same regime, the 'specific heat' (second derivative of the ground state energy with respect to λ^{-1}) appears to diverge rather strongly; the precise nature of the singularity is as yet unclear.

On the strong-coupling side, there is weak evidence from Padé analysis of the disorder parameter series for a strong-coupling boundary (shown dotted in figure 1) distinct from the weak-coupling boundary. Unfortunately, as noted above, it appears difficult to use finite-lattice methods in this regime.

(iii) $0.5 \leq \kappa \leq 1.1$

Here the evidence for two transitions is considerably stronger than for $0.35 \leq \kappa < 0.5$. Not only is the Padé analysis of the disorder parameter series more consistent, but these estimates are confirmed to within a few per cent by finite-size scaling of the mass gap. We are unable, however, to determine with any confidence how the disorder parameter vanishes at the strong-coupling boundary. Plots of the scaled finite-lattice mass gaps show some similarity to those obtained for the O(2) model (Hamer and Barber 1981, Roomany and Wyld 1980). This suggests that the transition is to a massless phase, in accord with an argument (Garel and Pfeuty 1976) that the transition is *XY*-like. However, our data are insufficient to allow a detailed analysis.

On the weak-coupling side, ratio analysis of the Γ_A series indicates a singularity at a *larger* value of λ than the strong-coupling boundary. Padé approximants are however very defective and the series too short to determine reliably the nature of the singularity. Padé approximants to Γ_A itself, when evaluated on the weak-coupling boundary, yield a rather consistent non-zero value. This could indicate that the transition is first-order.

(iv) $\kappa \geq 1.1$

Here the singularities in Γ_D and Γ_A agree to within the indicated precision and are supported by the finite-lattice results. The series analysis suggests that $\Gamma_D(\lambda, \kappa) \sim [1-\lambda/\lambda_c(\kappa)]^{1/4}$, in accord with (7), which holds at $\kappa = \infty$. Again the series for Γ_A is too short and its Padés too defective to determine reliably how Γ_A vanishes.

We conclude by briefly comparing our results with other recent work. The phase diagram, figure 1, has the same general topology as that found in Monte Carlo calculations (Selke and Fisher 1980). These were, however, restricted to $\kappa \leq 0.8$ and assumed isotropic nearest-neighbour intersections ($J_0 = J_1$), whereas our approach pertains to the extreme anisotropic limit (3). Rather significantly, both our results, the Monte Carlo calculations and the high-temperature susceptibility series (Redner, unpublished), indicate that something very definitely occurs at $\kappa \sim 0.35$. This could conceivably be consistent with a Lifshitz point. On the other hand, Villain and Bak (1981) and Coopersmith *et al* (1981) have argued that the ferromagnetic and floating phases do not co-exist but are always separated by a paramagnetic phase. In addition, Peschel and Emery (1981) have found a particular line along which the ground state energy and the correlation length can be determined exactly, the correlation length being everywhere finite. This line is shown in figure 1 and would appear to rule out a massless phase for $\kappa < \frac{1}{2}$. Our evidence for the transition in this region is very weak, yet the highly anomalous behaviour in Γ_F and the specific heat demands theoretical explanation. We know of no such explanation.

For $\kappa > \frac{1}{2}$, our results rather more strongly support the existence of a floating phase terminated by an upper Lifshitz point at a finite value of κ. Unfortunately, the nature of transitions in this regime remains unclear. Further theoretical as well as numerical calculations are desirable to resolve these questions.

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