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Continuous quantum phase transitions in the one-dimensional spin-1/2 axial next-nearest-neighbour Ising model in two orthogonal magnetic fields

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Abstract. We have investigated the one-dimensional spin-1/2 axial next-nearest-neighbour Ising (ANNNI) model in two orthogonal magnetic fields at zero temperature. There are four different possible ground state configurations for the ANNNI model in a longitudinal field, in the thermodynamic limit. The inclusion of a transverse field introduces quantum fluctuations which destroy the existing spin order along certain critical lines. The effects of the fluctuations in three of the four ordered regions were investigated using the finite-size scaling technique. The phase boundaries of the ANNNI model in two orthogonal magnetic fields were thus determined numerically. For certain limits of the Hamiltonian we compared the obtained results with the existing literature and our results were in good agreement with the results in the existing literature.

Keywords. Ising model; quantum phase transitions; axial next-nearest-neighbour Ising model; magnetic fields; exact diagonalization; finite-size scaling; spin systems.

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1. Introduction

Field-induced effects in low-dimensional quantum spin systems have been studied for a long time [1,2]. One should remark however that in the past, the longitudinal field was often introduced mainly as an artifice to facilitate the calculation of order parameter and associated susceptibility as can be seen in refs [3–5], and the transverse field to introduce quantum fluctuations [6,7]. Models incorporating two noncommuting fields are gaining popularity, however, among experimentalists as well as theoreticians as is evident in refs [8–11]. Sen [8] investigated the quantum phase transitions in the ferromagnetic transverse Ising model in a spatially modulated longitudinal field and obtained the phase diagram of the model at zero temperature, using finite-size scaling techniques. It was found that a continuous phase transition occurs everywhere except at the multiphase point $h_x = 0$ where a first-order transition exists. The values of the critical exponents obtained in ref. [8] are identical to those of the transverse Ising model, putting the model in the same universality class as the two-dimensional classical Ising model. Ovchinnikov *et al* [10] investigated the antiferromagnetic Ising chain in the presence of a transverse magnetic field and a longitudinal magnetic field, and showed that the quantum phase transition existing in the transverse Ising model remains in the presence of the longitudinal field. Using the density matrix renormalization group (DMRG) technique of [12], they found the critical line in the (h_x, h_z) plane where the mass gap disappears and the staggered magnetizations along the x- and z-axes vanish. The authors of ref. [10] established that the Ising model in two orthogonal magnetic fields belongs to the universality class of the transverse Ising model.

The main purpose of this article is to extend the model studied by Ovchinnikov *et al* [10], by including both nearest-neighbour and next-nearest-neighbour interactions. Our model is described by the Hamiltonian

$$H = H_z + H_x, \tag{1}$$

where

$$H_z = \sum_i S_i^z S_{i+1}^z + j \sum_i S_i^z S_{i+2}^z - h_z \sum_i S_i^z \tag{2a}$$

and

$$H_x = -h_x \sum_i S_i^x. \tag{2b}$$

h_x is the transverse field, h_z is the uniform longitudinal field, j is the next-nearest-neighbour exchange interaction, S_i are the usual spin-$\frac{1}{2}$ operators and the fields h_x and h_z are measured in units where the splitting factor and Bohr magneton are unity. j, h_x and h_z are all positive quantities and periodic boundary condition is assumed.

The organization of this paper is as follows: In §2 we examine the exactly solvable ANNNI model in a longitudinal field h_z and present its ground state diagram at zero temperature, in the thermodynamic limit. The zero temperature phase diagram of the one-dimensional ANNNI model in two orthogonal magnetic fields is obtained numerically in §3.

2. The longitudinal ANNNI model

The Hamiltonian H_z (eq. (2a)) describes the ANNNI model in a longitudinal field. This is a classical model, in the sense that the Hamiltonian is the sum of commuting quantities. At zero temperature, the structure of the ground state of (eq. (2a)) changes, depending on the choice of the parameters j and h_z, so that the model undergoes quantum phase transitions.

In the absence of next-nearest-neighbour interactions ($j = 0$), the model (eq. (2a)) reduces to the Ising model in a uniform longitudinal field

$$H_{j=0} = \sum_i S_i^z S_{i+1}^z - h_z \sum_i S_i^z \,, \tag{3}$$

which is exactly solvable, using the transfer matrix technique [13,14].

The model (3) is similar to the classical part of the Hamiltonian discussed in [8]. In fact, with a proper rescaling, the classical part of the model studied in ref. [8] can always be rewritten in the form of eq. (3). The ground state of the model (3) is antiferromagnetic for $h_z < 1$ and ferromagnetic for $h_z > 1$. The ground state is highly degenerate at $h_z = 1$.

The case $h_z = 0$ in eq. (2a) corresponds to the ANNNI chain

$$H_{h_z=0} = \sum_i S_i^z S_{i+1}^z + j \sum_i S_i^z S_{i+2}^z \,, \tag{4}$$

whose ground state is also well-known [13,15,16]. The ground state is antiferromagnetic for values of the next-nearest-neighbour exchange interaction $j < 1/2$ and the four-fold degenerate antiphase states $\uparrow\uparrow\downarrow\downarrow \cdots \uparrow\uparrow\downarrow\downarrow$ for $j > 1/2$. At $j = 1/2$ the ground state of the model (4) is infinitely degenerate with the degeneracy being equal to $\left((1+\sqrt{5})/2\right)^N$ for a chain of length N [4,16].

By extrapolation of the results of exact diagonalization of the one-dimensional ANNNI model in a uniform longitudinal field, we have obtained the ground state diagram of the model at zero temperature in the thermodynamic limit. Although this result is not new [17,18], we would like to emphasize that our approach is new and brings out the deep interconnectivity of the various symmetries (translation, space reflection and inversion) of the Hamiltonian (eq. (2a)). This will however be the subject of another paper and will not be pursued here. We merely present the phase diagram (figure 1), since it is essential to the understanding of the effects of the transverse field on the ANNNI model in a field, the subject matter of the present article.

3. Phase transitions

We have employed the finite-size scaling ansatz to determine the critical points $(h_{x_\mathrm{C}}, h_{z_\mathrm{C}})$ for fixed j and $(h_{x_\mathrm{C}}, j_\mathrm{C})$ for fixed h_z for the one-dimensional ANNNI model in two orthogonal magnetic fields, described by the Hamiltonian (1)

$$H = \sum_{i=1}^N S_i^z S_{i+1}^z + j \sum_{i=1}^N S_i^z S_{i+2}^z - h_x \sum_{i=1}^N S_i^x - h_z \sum_{i=1}^N S_i^z .$$

The method introduced by the authors of ref. [19] and later developed and generalized by the authors of ref. [20] has turned out to be a valuable tool in evaluating critical behaviour from numerical results by extrapolating information obtained from a finite system to the thermodynamic limit [21,22]. The technique gives reliable results for different models and different types of critical behaviour [21].

A list of references on numerous successful applications of the finite-size scaling technique (at nonzero temperature) to various models is found in ref. [21].

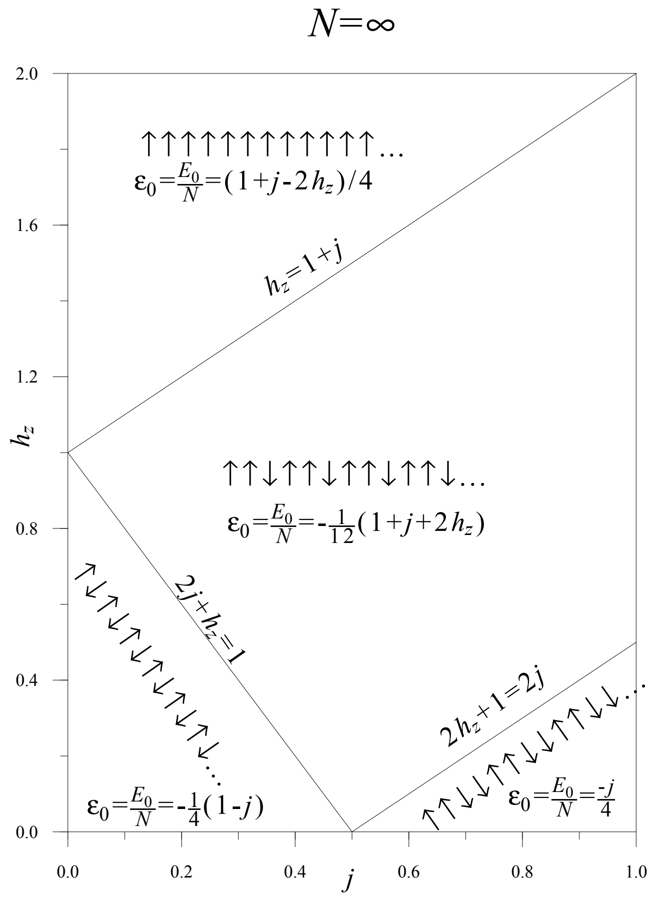

Figure 1. $T = 0$ phase diagram of the longitudinal ANNNI model: $H_z = \sum_i S_i^z S_{i+1}^z + j \sum_i S_i^z S_{i+2}^z - h_z \sum_i S_i^z$.

The finite-size scaling technique is also gaining popularity in the study of quantum phase transitions (that is, phase transitions at zero temperature) that are driven by competition and quantum fluctuations alone, as opposed to conventional, thermally-driven phase transitions. The author of ref. [8] employed finite-size scaling technique to investigate the quantum phase transitions in the Ising model in spatially modulated field and obtained the ferromagnetic-to-paramagnetic phase transition diagram of the model. The model was found to belong to the universality class of the two-dimensional Ising model. In ref. [22], the finite-size scaling was employed directly (that is, without making explicit analogy to classical statistical mechanics) to study the critical behaviour of quantum Hamiltonians. The authors also reported their success in an earlier study where the critical charges for two- and three-electron atoms were obtained by combining finite-size scaling with transfer matrix calculations of a classical pseudosystem.

3.1 *Finite-size scaling ansatz*

The basic equation for finite-size scaling is

$$N\Delta E_N = N'\Delta E_{N'}\,, \tag{5}$$

with

$$\Delta E_N = E_N^1(j, h_x, h_z) - E_N^0(j, h_x, h_z)\,. \tag{6}$$

N and N' are different system sizes, E_N^0 and E_N^1 respectively are the ground state energy and the energy of the first excited state of the model which are functions of the parameters j, h_x and h_z. The energy gap ΔE_N is related to the inverse correlation length of the classical model.

In considering quantum fluctations introduced by the transverse field h_x, for two different system sizes N and N', j and h_z are kept fixed and one keeps adjusting (refining) h_x until eq. (5) is satisfied to the desired accuracy. This value of h_x is then the critical value of the transverse field.

The correlation critical exponent, ν, is estimated from the following formula:

$$\nu = \frac{N}{N'}\frac{\partial\Delta E_N/\partial h_x}{\partial\Delta E_{N'}/\partial h_x}\,. \tag{7}$$

The partial derivatives are evaluated at the critical value of h_x for given j and h_z.

We stress here the point that we have investigated the different phases in relation to the magnetic fields always at temperature $T = 0$. We took advantage of the translational symmetry of the Hamiltonian under periodic boundary conditions to drastically reduce the dimensions of the Hilbert space of the spin systems in the total S_z basis. The Hamiltonian H was diagonalized in the orthogonal subspaces of the translation operator. A maximum system size of 12 spins was considered. The matrix of H in each subspace was generated by Maple and diagonalized by Matlab. The source code for the numerical implementation is available from the authors upon request. Considering the high accuracy which is characteristic of the finite-size scaling technique [21], we believe that $N = 12$ is adequate to produce reliable results. In fact, fewer or comparable systems have been treated in the recent past [8,23]. There is no doubt, of course, that more accurate results will be obtained by diagonalizing larger systems, only that this is computationally more involving and at any rate will not lead to remarkable qualitative improvement in the diagrams. The fact that we were able to reproduce results of the known limits of Hamiltonian (1) also support this point and is also an indication that our results for the general model (1) are correct.

We see from the phase diagram of the one-dimensional ANNNI model in a longitudinal field (figure 1), that there are four different ground state configurations of the model in the absence of the transverse field h_x. We have investigated the effect of the quantum fluctuations introduced by the perpendicular field on the existing order in three of the four regions, excluding the ferromagnetic region, and our findings are reported below.

One of the reasons our model (1) is interesting to study is the fact that it is an embodiment of various models (depending on the choice of j, h_x and h_z). Some

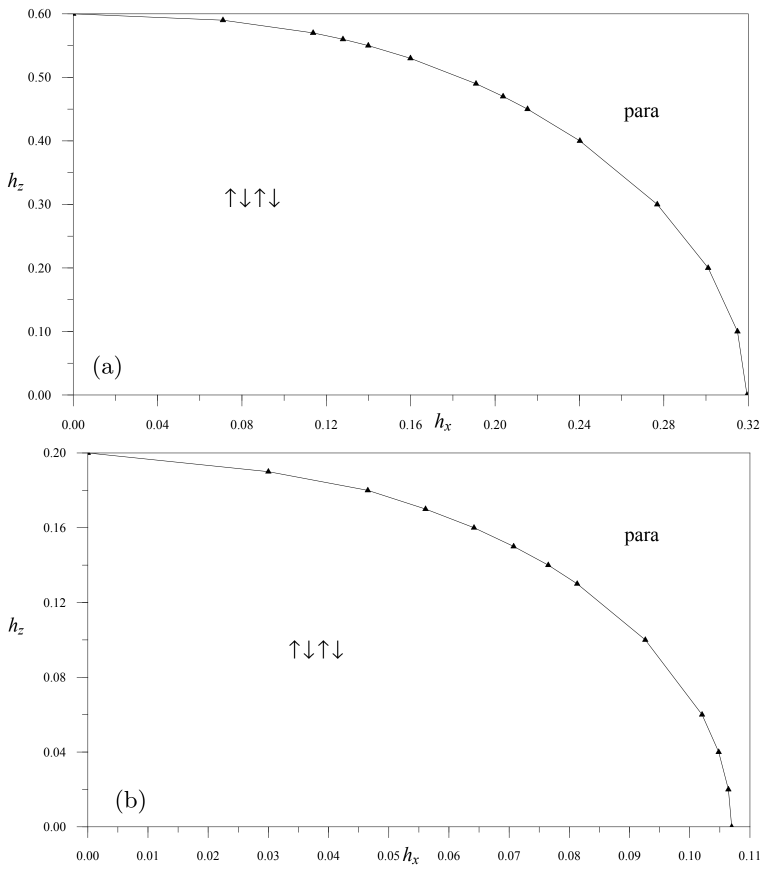

Figure 2. Phase boundary between antiferromagnetic and paramagnetic regions for the one-dimensional ANNNI model in mixed longitudinal field h_z and transverse field h_x. (**a**) Critical line between antiferromagnetic phase and paramagnetic phase for $j = 0.2$. (**b**) Critical line between antiferromagnetic phase and paramagnetic phase for $j = 0.4$.

of these models are exactly solvable (for example, the Ising model in a transverse field, corresponding to $j = 0 = h_z$ and the ANNNI model ($h_x = h_z = 0$)), while the phase diagrams of the others (the ANNNI model in a transverse field or the model studied in ref. [10] for example) can only be estimated using approximation techniques. We applied the finite-scaling technique to obtain the phase diagram of our model, Hamiltonian (1) (the ANNNI model with two orthogonal magnetic fields). In addition to our new results, we were also able to verify the ones known in the literature.

3.1.1 *The antiferromagnetic ANNNI model in two orthogonal magnetic fields*

The main motivation for this work was supplied by the investigations carried out in [10], the model therein corresponding to $j = 0$ in our model. What we have

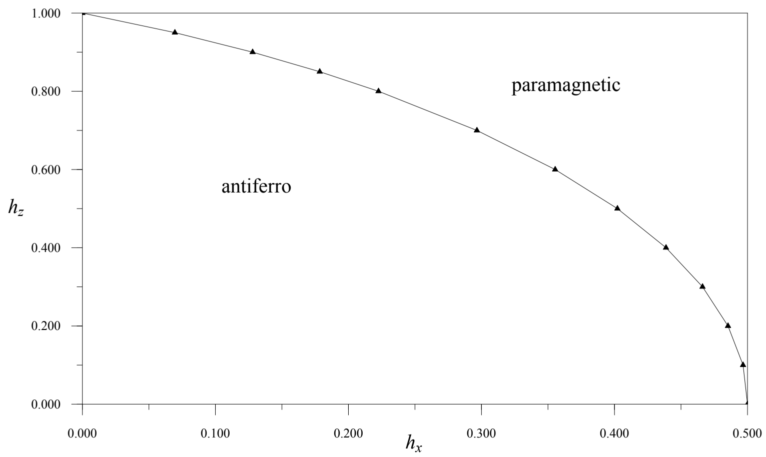

Figure 3. Phase boundary separating the paramagnetic from the antiferromagnetic states for $j = 0$.

done was to extend the investigation in [10] by including next-nearest-neighbour interactions. We investigated the Hamiltonian (1) for $j = 0.2$ and 0.4. For $j = 0.2$, we applied the scaling ansatz for $0 < h_z < 0.6$ (keeping within the constraint $2j + h_z < 1$). Equation (5) then becomes

$$N\Delta E_N(0.2, h_x, h_z) = N'\Delta E_{N'}(0.2, h_x, h_z). \tag{8}$$

For each value of h_z, the value of h_x for which the above equation is satisfied for given N and N' was determined. We thus obtain a collection of points (h_{x_C}, h_{z_C}). This scheme was repeated for $j = 0.4$ for $0 < h_z < 0.2$.

In each case the critical line separating the antiferromagnetic phase from the paramagnetic phase was obtained. The resulting phase diagrams for $j = 0.2$ and 0.4 based on the collection of critical points (h_x, h_z) from finite-size scaling are displayed in figure 2. In both cases the transition is from the ordered antiferromagnetic to the paramagnetic phase.

There is no qualitative difference in the phase diagrams for $j = 0.2$ and 0.4 and that of the model studied in ref. [10] (corresponding to $j = 0$, figure 3). The effect of the next-nearest-neighbour interactions turned out to be simply to shrink the antiferromagnetic region. This is probably not surprising since in the absence of the perpendicular field h_x, the ground state of Hamiltonian (1) is antiferromagnetic in the region $2j + h_z < 1$ as can be seen from the $h_x = 0$ phase diagram. It must be emphasized that only when $2j + h_z < 1$ does the inclusion of the next-nearest-neighbour interaction not lead to new physical effects (figure 3). The para to up-up-down boundary in figures 4 and 5 are new physical effects and they occur only at finite j.

Table 1. Critical field and the corresponding critical exponent for the phase boundary of the ANNNI model in two orthogonal magnetic fields.

j	h_{x_C}	ν
0	0.48518	1.07281
0.1	0.397037	1.064492
0.2	0.30105	1.042743
0.3	0.19032	0.964838
0.5	0.265	0.907053
0.6	0.39016	1.0762272
0.7	0.498	1.191895

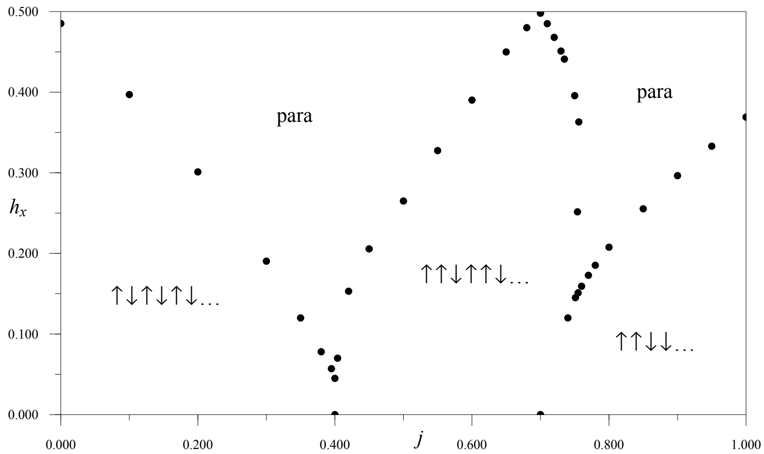

Figure 4. $T = 0$ phase diagram of the ANNNI model in two orthogonal magnetic fields for $h_z = 0.2$.

3.1.2 *The general ANNNI model in two orthogonal magnetic fields*

The ANNNI model in two orthogonal magnetic fields h_x and h_z can also be viewed as the transverse ANNNI model in a longitudinal field h_z. This approach is useful because estimates of the phase boundaries of the transverse ANNNI model ($h_z = 0$) have already been obtained in refs [23,24]. The investigation here is then to observe the effect of the presence of a finite longitudinal field h_z on the phases. There are three main regions in the phase diagram of the transverse ANNNI model – the ordered antiferromagnetic region, the paramagnetic region and the ordered period-4 $\langle 2 \rangle$ antiphase region as shown in figure 6. What we have done was to gradually switch on the longitudinal field h_z. The results for $h_z = 0.2$ and 0.5 presented below are typical.

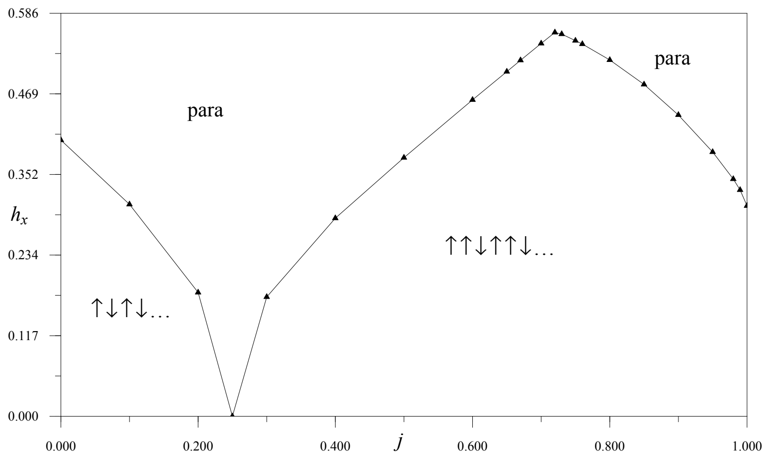

Figure 5. $T = 0$ phase diagram of the ANNNI model in two orthogonal magnetic fields for $h_z = 0.5$.

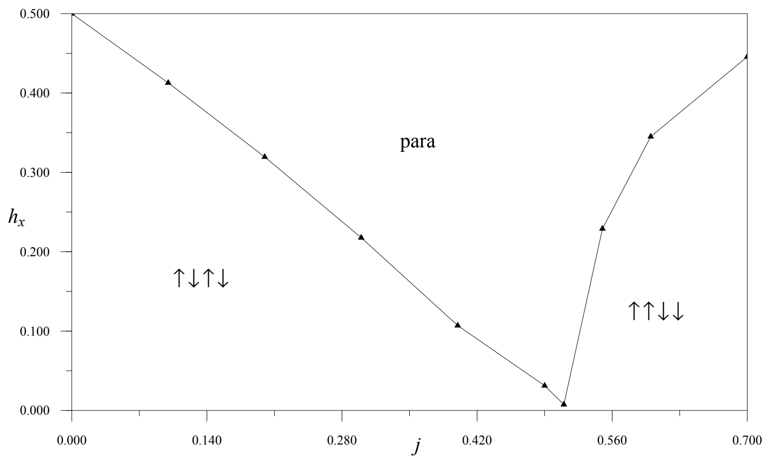

Figure 6. $T = 0$ phase diagram of the transverse ANNNI model.

(a) $h_z = 0.2$

Here the finite-size scaling ansatz is

$$N\Delta E_N(j, h_x, 0.2) = N'\Delta E_{N'}(j, h_x, 0.2)\,. \tag{9}$$

The introduction of a finite external longitudinal field h_z alters the phase diagram of the transverse ANNNI model in a significant way. A third ordered phase appears and the phase diagram becomes richer. First the antiferromagnetic order gives way to the disordered paramagnetic region. Order begins to set in again as j is increased beyond 0.4 (for $h_z = 0.2$) and the new ground state is the period 3 ↑↑↓↑↑↓ spin configuration. For low values of the field h_x the period 3 ground state order disappears and antiphase order appears. For relatively high values of h_x however, there is a small paramagnetic area between the period 3 phase and the period 4 antiphase ground state as can be seen in figure 4.

The critical exponents were calculated, using (7) and tabulated in table 1. From the table $\nu \approx 1$, so that the ANNNI model in two orthogonal magnetic fields is still in the same universality class as the zero-field classical two-dimensional ANNNI model. The phase diagram obtained from the finite-size scaling data points is shown in figure 4.

The richness of the phase diagram is not surprising when one examines the phase diagram of the one-dimensional ANNNI model in longitudinal field. The ground state is the two-fold degenerate antiferromagnetic state for $2j + h_z < 1$, the four-fold degenerate antiphase states for $2h_z + 1 < 2j$, and the period-3 $\uparrow\uparrow\downarrow\uparrow\uparrow\downarrow \cdots$ in the region bounded by the lines $2j + h_z < 1$ and $2h_z + 1 < 2j$ in the h_z–j plane. Thus in the absence of the longitudinal field ($h_z = 0$, transverse ANNNI model), only the antiferromagnetic order (for $j < 0.5$) and the antiphase order (for $j > 0.5$) exist. In this situation the frustration introduced by the presence of the transverse field destroys the antiferromagnetic order for $j < 0.5$ while, as the next-nearest-neighbour interactions become stronger ($j > 0.5$) the competition combines with the frustration to produce a new order, the antiphase alignment. For a finite longitudinal field h_z however, there is the additional period-3 ground state structure to consider.

As far as the estimation of continuous phase boundaries is concerned therefore, the exact solvability of the longitudinal ANNNI model already gives one a rough idea of what to expect in the presence of quantum fluctuations. The main point is then the accurate determination of the transition lines, a task which the finite-size scaling technique handles very well.

(b) $h_z = 0.5$

The scaling ansatz is

$$N\Delta E_N(j, h_x, 0.5) = N'\Delta E_{N'}(j, h_x, 0.5)\,. \tag{10}$$

Increasing the strength of the longitudinal field h_z to 0.5 produced an interesting effect on the phase diagram of the ANNNI model in mixed fields. It became possible to determine accurately the phase boundary where the period-3 ground state structure disappears. This can be easily seen in the phase diagram shown in figure 5 where around $j > 0.7$ the critical line takes a downward turn. The convergence and smoothness of the data points indicate that this is clearly a second-order phase transition. This however does not rule out the possibility of the existence of floating phases in the region as well. The existence or otherwise of such phases will have to be investigated using other means.

4. Known limits of the Hamiltonian (1)

As mentioned earlier, various limits of our model are exactly solvable while the phase diagrams of the others have been estimated using various approximation techniques. In addition to our new results, we were also able to verify the ones known in the literature, as presented below.

4.1 *The transverse Ising model*

With $j = 0 = h_z$ in the Hamiltonian (1), the resulting Hamiltonian is

$$H = \sum_i S_i^z S_{i+1}^z - h_x \sum_i S_i^x, \tag{11}$$

which describes the one-dimensional Ising model in a transverse field h_x. The model (11), an exactly solvable one-dimensional model, is well studied. At zero temperature, the antiferromagnetic order in the ground state is destroyed at $h_x = 0.5$ [6,10]. An application of the finite-size scaling ansatz

$$N\Delta E_N(0, h_x, 0) = N'\Delta E_{N'}(0, h_x, 0) \tag{12}$$

confirms this result, giving the critical value of $h_x = 0.5002$ with the critical exponent $\nu = 1.074$ (compared with the exact value of $\nu = 1$).

4.2 *The Ovchinnikov model*

Next we applied the finite-size scaling ansatz to another model whose phase diagram has been obtained: the antiferromagnetic Ising model in the presence of two mutually perpendicular fields, described by the Hamiltonian

$$H = \sum_i S_i^z S_{i+1}^z - h_x \sum_i S_i^x - h_z \sum_i S_i^z. \tag{13}$$

This model corresponds to our model without next-nearest-neighbour spin interactions, that is $j = 0$ in the Hamiltonian (1). The authors of ref. [10] carried out density matrix renormalization group (DMRG) calculations and obtained the critical line of the model. The authors also concluded that the antiferromagnetic Ising model in a mixed field is in the same universality class as the classical two-dimensional Ising model. Our finite-size scaling results reproduced the phase diagram for this model, as expected. The scaled mass gap is plotted in figure 7 while the resulting phase diagram for $j = 0$, based on the collection of points (h_{x_C}, h_{z_C}) is displayed in figure 3.

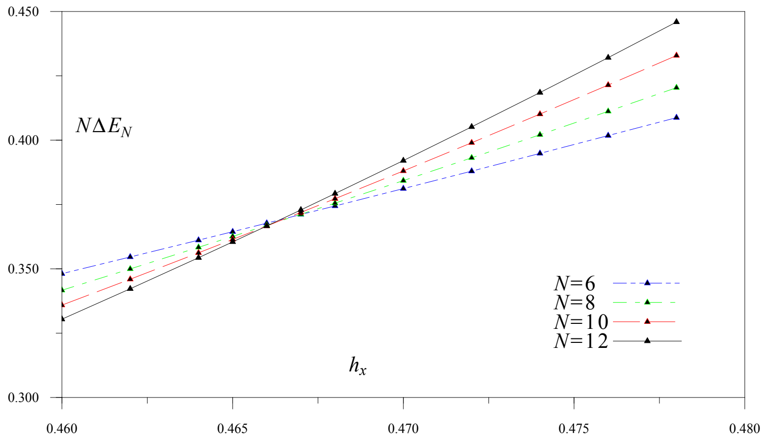

Figure 7. Typical scaled mass gap for various system sizes for $j = 0$. The points shown here are taken at $h_z = 0.3$. The point of intersection gives the critical point h_{x_C}.

4.3 *The ANNNI model in a transverse field:* $h_z = 0$

The one-dimensional transverse ANNNI model is another model whose phase diagram has been obtained using various methods. Arizmendi *et al* [25] used Monte Carlo simulations to obtain the continuous phase boundary separating the ferromagnetic states from the paramagnetic phase, and that separating the paramagnetic states from the four-fold degenerate $\langle 2 \rangle$ antiphase states. Sen [26] applied the interface approach to the model and obtained similar diagrams. There were also speculations concerning the existence of floating phases close to the antiphase regions [26,27]. Implementing the DMRG algorithm for entanglement entropy calculations, Beccaria *et al* [28] obtained clear evidence for the existence of a floating phase for $j > 0.5$, extending at least up to $j = 5$. It however remains an open question whether the floating phase extends up to $j = \infty$. Guimarães *et al* [23] employed the finite-size scaling technique to obtain the second-order phase transitions in the same model. We remark that all the above references investigated the ferromagnetic model. We have applied the finite-size scaling technique to obtain the phase diagram of the antiferromagnetic ANNNI model in a transverse field. The Hamiltonian is given by $h_z = 0$ in eq. (1), that is

$$H = \sum_i S_i^z S_{i+1}^z + j \sum_i S_i^z S_{i+2}^z - h_x \sum_i S_i^x. \tag{14}$$

The application of an external magnetic field h_x destroys the existing antiferromagnetic order which exists for $j < 0.5$ in zero field. The critical line between the antiferromagnetic phase and the disordered states was obtained. As j is increased beyond 0.5 under the influence of the external perpendicular field h_x, the ground state of the system became ordered and the continuous transition line separating the paramagnetic phase from the antiphase region was also determined. The phase diagram of the antiferromagnetic ANNNI model in a transverse field based on the finite-size scaling data points is exhibited in figure 6. It may be observed that in the difficult region of $j > 0.5$, there is some variation in our phase diagram and that obtained by earlier researchers, (e.g. the Monte Carlo results of Arizmendi *et al* [25] and the finite-size scaling of Williams *et al* [21] and Guimarães *et al* [23]). It must however be remembered that the earlier results are based on data from fewer ($\leq$8) spin sites. As noted earlier, the existence of a floating phase in the region $j > 0.5$ has been confirmed by Beccaria *et al* [28] (at least for the ferromagnetic model). The finite-size scaling technique as used in our investigation is incapable of determining first-order transition lines.

5. Conclusion

We have investigated the one-dimensional spin-1/2 ANNNI model in two orthogonal magnetic fields h_x and h_z. The case $j = 0$, $h_z < 1$ has already been investigated in ref. [10], where the critical line between the antiferromagnetic phase and the paramagnetic phase was obtained. Things got more interesting following the introduction of next-nearest-neighbour interactions through the finite exchange integral j. Next-nearest-neighbour interactions increased the number of zero temperature ground state configurations in $h_x = 0$ from one in ref. [10] to four in this present study. The spin order in each of the three regions considered here was found to be destroyed by quantum fluctuations introduced by the transverse field h_x. The critical lines were accurately determined using the finite-size scaling method. It is interesting to emphasize that while there is no qualitative difference between the phase diagram for $j = 0$ and that for finite j in the antiferromagnetic region ($2j + h_z < 1$), the next-nearest-neighbour interactions did introduce additional ordered regions, in addition to the antiferromagnetic phase, for finite values of the longitudinal field h_z. Since the finite-size scaling technique does not directly detect the existence of floating phases, the presence of the same in the one-dimensional ANNNI model will have to be investigated using other means. The phase diagrams presented in this paper describe only second-order phase transitions. A workaround has been suggested by Xavier *et al* [29] which will make it possible to also estimate first-order transitions. The entanglement entropy method used by Beccaria *et al* [28] is also another possibility. Our second-order phase transition diagrams for the ANNNI model in two orthogonal magnetic fields at absolute zero are as presented in figures 4 and 5.

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