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Perturbation Expansions of the Ground State Energy of the Antiferromagnetic ANNNI Model in Two Perpendicular External Magnetic Fields

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ABSTRACT

Using Rayleigh-Schrödinger perturbation theory, we derive analytic expressions for the ground state energy of the antiferromagnetic Axial Next Nearest Neighbour Ising (ANNNI) model in two mutually orthogonal external magnetic fields. Expressions for various physical quantities are also derived. The calculations are carried out to the fourth order in the transverse field.

Keywords: Perturbation expansions, ANNNI model, magnetic fields, order parameters

INTRODUCTION

Hamiltonian spin models incorporating two external mutually orthogonal magnetic fields are being increasingly studied these days [1, 2, 3]. An example of such a model is the one dimensional spin 1/2 antiferromagnetic Axial Next Nearest Neighbour Interaction (ANNNI) model in the presence of a perpendicular external magnetic field h_x and a longitudinal field h_z , described by the Hamiltonian

$$\begin{split} H &= \sum_{i} S_{i}^{z} S_{i+1}^{z} + j \sum_{i} S_{i}^{z} S_{i+2}^{z} - h_{z} \sum_{i} S_{i}^{z} - h_{x} \sum_{i} S_{i}^{x} \\ &= H_{z} + H_{x}, \end{split}$$

where

$$H_{z} = \sum_{i} S_{i}^{z} S_{i+1}^{z} + j \sum_{i} S_{i}^{z} S_{i+2}^{z} - h_{z} \sum_{i} S_{i}^{z}$$
(1)

and

Here *j* is the next nearest neighbour exchange interaction, S_i are the usual spin-1/2 operators and the fields h_x and h_z are measured in units where the splitting factor and Bohr magneton are unity.

 $H_x = -h_x \sum_i S_i^x \, .$

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(2)

The model described by the Hamiltonian H cannot be solved exactly, as is almost always the case with such models. It is therefore often necessary to resort to approximate solution techniques, perturbation being a convenient and useful choice. The (sub)Hamiltonian H_z , describing the ANNNI model in a longitudinal field is diagonal in both the total S_z basis as well as in the eigenbases of the orthogonal subspaces of the translation operator [4], T. Thus it is convenient to treat $H_x = -h_x \sum_i S_i^x$ as a perturbation on Hz for $h_x < 1$. The ground state of H_z is antiferromagnetic in the region bounded by $2j + h_z < 1$, the non-degenerate ferromagnetic state in the region bounded by $2h_z + 1 = 2j$ and the j axis, and the three-fold degenerate $\uparrow\uparrow\downarrow$ in the region bounded by the three lines $2h_z + 1 = 2j$, $2j + h_z < 1$ and $h_z = 1 + j$. All this information is contained in figure 1.



Figure 1: Ground state energy diagram of the longitudinal ANNNI model, H_z

In this paper we will assume, without any loss of generality, that the number of spins N is a multiple of 12. Periodic boundary condition is also assumed, so that $S_{N+1}^{x(z)} = S_1^{x(z)}$ and $S_{N+2}^{x(z)} = S_2^{x(z)}$.

In section 2 we will investigate the effect of h_x on the longitudinal ANNNI model in the region $2j + h_z < 1$. In section 3 we apply the perturbation treatment to the ferromagnetic ground state. In section 4, similar investigations will be made for the antiphase ground states, while the perturbation effects on the $\uparrow\uparrow\downarrow$ states will be examined in section 5

2 The antiferromagnetic ground state

We will denote the two-fold degenerate antiferromagnetic states of H_z in the region $2j + h_z < 1$ by the total S_z direct product states $|AF^+\rangle$ and $|AF^-\rangle$, where

$$\begin{aligned} \left| AF^{+} \right\rangle &= \left| \uparrow \right\rangle \otimes \left| \downarrow \right\rangle \otimes \left| \uparrow \right\rangle \otimes \left| \downarrow \right\rangle \cdots \left| \uparrow \right\rangle \otimes \left| \downarrow \right\rangle \otimes \left| \downarrow \right\rangle \otimes \left| \downarrow \right\rangle \\ &= \left| \uparrow \downarrow \uparrow \downarrow \cdots \uparrow \downarrow \uparrow \downarrow \right\rangle \end{aligned}$$
(3)

and

$$\begin{vmatrix} AF^{-} \rangle &= |\downarrow\rangle \otimes |\uparrow\rangle \otimes |\downarrow\rangle \otimes |\uparrow\rangle \cdots |\downarrow\rangle \otimes |\uparrow\rangle \otimes |\downarrow\rangle \otimes |\uparrow\rangle \\ &= |\downarrow\uparrow\downarrow\uparrow\cdots\downarrow\uparrow\downarrow\downarrow\rangle$$

$$(4)$$

The degenerate antiferromagnetic ground state energy is

$$E_{AF^{+}}^{(0)} = E_{AF^{-}}^{(0)} = -\frac{N}{4}(1-j).$$
(5)

In order to facilitate the calculation of physical quantities like the order parameter and the associated susceptibility, we introduce a field $\alpha > 0$ and write the unperturbed Hamiltonian H_z (1) as

$$H_{z} = \sum_{i=1}^{N} S_{i}^{z} S_{i+1}^{z} + j \sum_{i=1}^{N} S_{i}^{z} S_{i+2}^{z} - h_{z} \sum_{i=1}^{N} S_{i}^{z} - \alpha \sum_{i=1}^{N/2} (S_{2i-1}^{z} - S_{2i}^{z}).$$
(6)

This way, it will then be possible to compute the long range antiferromagnetic order (staggered magnetization) ρ_{AF} and the susceptibility χ_{AF} from

$$\rho_{AF} = -\frac{2}{N} \frac{\partial E_{AF}(\alpha)}{\partial \alpha} \bigg|_{\alpha=0}$$
(7)

and

$$\chi_{AF} = -\frac{2}{N} \frac{\partial^2 E_{AF}(\alpha)}{\partial \alpha^2} \bigg|_{\alpha=0} .$$
(8)

We note that the introduction of α breaks the translational invariance symmetry and thus removes the ground state degeneracy, now giving

$$E_{AF^{\pm}}^{(0)} = -N(1-j\pm 2\alpha)/4,$$
(9)

with $E_{AF^+}^{(0)}$ being the non-degenerate ground state energy belonging to the state $|AF^+\rangle = |\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow\cdots\uparrow\downarrow\rangle$.

2.1 Energy corrections

2.1.1 First order correction

Since the degeneracy remains at $\alpha = 0$ we will apply degenerate perturbation theory to obtain the corrections to the ground state energy.

The operator $H_x = -\sum_{i=1}^{N} S_i^x$, acting on an eigenstate of total S_z generates a linear combination of N states with the *i*th spin flipped in the *i*th member, with each spin flip costing ±1 in the total S_z quantum number of the *i*th member state. This means that a necessary (but not sufficient) condition for the matrix element of H_x between any two states $|a\rangle$ and $|b\rangle$ not to vanish is that the absolute value of the total S_z quantum number of $|a\rangle$ and that of $|b\rangle$ must be 1. That is

$$\langle b | H_x | a \rangle = 0 \tag{10}$$

whenever
$$|S_z(|a\rangle) - S_z(|b\rangle)| \neq 1,$$
 (11)

where $|a\rangle$ and $|b\rangle$ are eigenstates of total S_z . In particular

$$\langle a | H_x | a \rangle = 0 \tag{12}$$

for any $|a\rangle$ an eigenstate of S_z .

To first order in h_x , the perturbation matrix, V, of H_x is

$$V = \begin{pmatrix} \left\langle AF^{+} \left| H_{x} \right| AF^{+} \right\rangle & \left\langle AF^{+} \left| H_{x} \right| AF^{-} \right\rangle \\ \left\langle AF^{-} \left| H_{x} \right| AF^{+} \right\rangle & \left\langle AF^{-} \left| H_{x} \right| AF^{-} \right\rangle \end{pmatrix},$$
(13)

and since both $|AF^+\rangle$ and $|AF^-\rangle$ are total $S_z = 0$ states, it follows from (10) that V is a null matrix, so that there is no first order correction to the antiferromagnetic ground state energy.

2.1.2 Second order correction

The 2×2 perturbation matrix for the second order correction to the ground state energy has elements

$$V_{11} = \sum_{m} \frac{\langle AF^{+} | H_{x} | m \rangle \langle m | H_{x} | AF^{+} \rangle}{E_{AF}^{(0)} - E_{m}^{(0)}},$$

$$V_{12} = \sum_{m} \frac{\langle AF^{+} | H_{x} | m \rangle \langle m | H_{x} | AF^{-} \rangle}{E_{AF}^{(0)} - E_{m}^{(0)}},$$

$$V_{21} = \sum_{m} \frac{\langle AF^{-} | H_{x} | m \rangle \langle m | H_{x} | AF^{+} \rangle}{E_{AF}^{(0)} - E_{m}^{(0)}},$$
and
$$V_{22} = \sum_{m} \frac{\langle AF^{-} | H_{x} | m \rangle \langle m | H_{x} | AF^{-} \rangle}{E_{AF}^{(0)} - E_{m}^{(0)}}.$$
(14)

Each of the summations over m above extends over the total S_z direct-product basis states $|m\rangle$

of the Hamiltonian, but excluding the states $|AF^+\rangle$ and $|AF^-\rangle$.

By inspection of the definitions (4), it is clear that any state whose H_x matrix element with $|AF^-\rangle$ does not vanish must have a vanishing matrix element with $|AF^+\rangle$ and vice versa.

That is

$$\left\langle AF^{-} \left| H_{x} \right| m \right\rangle = 0 \text{ whenever} \left\langle AF^{+} \left| H_{x} \right| m \right\rangle \neq 0$$

and $\left\langle AF^{+} \left| H_{x} \right| m \right\rangle = 0 \text{ whenever} \left\langle AF^{-} \left| H_{x} \right| m \right\rangle \neq 0$ (15)

for any $|m\rangle$ in the Hilbert space of H.

The conditions in (15) imply that the off-diagonal matrix elements V_{12} and V_{21} are zero.

In V_{11} , there are only N non-vanishing matrix elements $\langle m | H_x | AF^+ \rangle$ contributed by states $| m \rangle$ such that

$$|m\rangle \in \left\{ \downarrow \downarrow \uparrow \downarrow \uparrow \downarrow \cdots \uparrow \downarrow \rangle, |\uparrow \uparrow \uparrow \downarrow \uparrow \downarrow \cdots \uparrow \downarrow \rangle, \cdots, |\uparrow \downarrow \uparrow \downarrow \cdots \uparrow \uparrow \rangle \right\}.$$
(16)

N/2 of these states (corresponding to N/2-1 configurations with 3 consecutive spins down and 1 configuration with first two spins up and the last spin up, with total $S_z(|m\rangle) = -1$) contribute

$$\frac{N}{2}\frac{h_x^2}{4}\frac{-1}{1-j+\alpha+h_z}$$
(17)

to V_{11} while N/2 states (corresponding to N/2-1 states with 3 consecutive spins up and 1 configuration with first two spins down and the last spin down, with total $S_z(|m\rangle) = +1$) contribute

$$\frac{N}{2}\frac{h_x^2}{4}\frac{-1}{1-j+\alpha-h_z}.$$
(18)

The diagonal element V_{11} therefore evaluates to

$$V_{11} = -\frac{Nh_x^2}{8} \left(\frac{1}{1 - j + \alpha + h_z} + \frac{1}{1 - j + \alpha - h_z} \right).$$
(19)

Similarly, we have

$$V_{22} = -\frac{Nh_x^2}{8} \left(\frac{1}{1 - j - \alpha + h_z} + \frac{1}{1 - j - \alpha - h_z} \right).$$
(20)

In the limit $\alpha \to 0$, V_{11} and V_{22} give the second order corrections to the antiferromagnetic ground state energy to be

$$E_{AF^{+}}^{(2)} = E_{AF^{-}}^{(2)} = -\frac{Nh_{x}^{2}}{8} \left(\frac{1}{1-j+h_{z}} + \frac{1}{1-j-h_{z}} \right)$$
$$= -\frac{Nh_{x}^{2}}{4} \frac{(1-j)}{(1-j)^{2}-h_{z}^{2}}.$$
(21)

We see that, to second order in perturbation, the degeneracy in the ground state energy is not lifted by the application of an external magnetic field h_x . This is probably a manifestation of the translational invariance which exists for $\alpha = 0$. Translation invariance is a symmetry of our general Hamiltonian, even in the presence of an external transverse magnetic field. One should therefore expect the two-fold degeneracy of the antiferromagnetic states to remain to any order in perturbation. This is in fact known to be the case in the thermodynamic limit, at least for the transverse Ising model ($j = 0 = h_z$) for $h_x < 0.5$ [3].

As expected, the second order correction to the ground state energy (equation (21)) is negative since 1-j > 0 (because $2j+h_z < 1$) and $(1-j)^2 - h_z^2 = (1-j-h_z)(1-j+h_z)$ is clearly a positive quantity in the region $2j-h_z < 1$ for which the perturbation is carried out $(2j+h_z < 1 \Rightarrow 1-j > j+h_z \Rightarrow 1-j > \pm h_z$ since $j, h_z > 0$).

From (5) and (21) we have that the antiferromagnetic ground state energy to second order in h_x is given by

$$E_{AF} = -\frac{N(1-j)}{4} \left(1 + \frac{h_x^2}{(1-j)^2 - h_z^2} \right).$$
(22)

So that the antiferromagnetic ground state energy per spin is

$$\varepsilon_{AF} = -\frac{(1-j)}{4} \left(1 + \frac{h_x^2}{(1-j)^2 - h_z^2} \right).$$
(23)

From (9) and (19) we have

$$E_{AF^{+}}(\alpha) = -\frac{N(1-j+2\alpha)}{4} - \frac{Nh_{x}^{2}}{4} \frac{1-j+\alpha}{(1-j+\alpha)^{2} - h_{z}^{2}},$$
(24)

where for the sake of definiteness we have taken $|AF^+\rangle = |\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow\cdots\uparrow\downarrow\rangle$ as the definition of the antiferromagnetic ground state. Results for $|AF^-\rangle$ can be obtained from those for $|AF^+\rangle$ by replacing α with $-\alpha$.

The staggered magnetization is then obtained as

$$\rho_{AF^{+}} = -\frac{2}{N} \frac{\partial}{\partial \alpha} \left(E_{AF^{+}}(\alpha) \right)_{\alpha=0}$$

= $1 + \frac{1}{2} \frac{h_{x}^{2}}{(1-j)^{2} - h_{z}^{2}} \left(1 - \frac{2(1-j)}{(1-j)^{2} - h_{z}^{2}} \right).$ (25)

We observe that

$$\frac{(1-j)}{(1-j)^2 - h_z^2} = \frac{1}{1-j} \left(\frac{1}{1 - \frac{h_z}{(1-j)^2}} \right) > 1,$$
(26)

so that $\rho_{AF^+} < 1$ which is consistent with the requirement that the staggered magnetization attain its maximum value of unity in zero external transverse field.

The magnetic susceptibility is obtained from equation (8) as

$$\chi_{AF^{+}} = -\frac{h_{x}^{2}(1-j)}{((1-j)^{2} - h_{z}^{2})^{2}} \left(3 - \frac{4(1-j)^{2}}{(1-j)^{2} - h_{z}^{2}}\right).$$
(27)

We notice that the bracketed term is always negative, which means that χ_{AF^+} is always a positive quantity. This is consistent with the inequality proved by Ferrell [5, 6] for a Hamiltonian with a linear dependence on a parameter λ for the ground state energy, namely that

$$\frac{\partial^2 E}{\partial \lambda^2} \le 0. \tag{28}$$

2.1.3 Third order correction

The third order correction to the ground state energy contains terms of the form

$$E_{AF^{+}}^{(3)} = \sum_{k,m} \frac{\langle AF^{+} | H_{x} | m \rangle \langle m | H_{x} | k \rangle \langle k | H_{x} | AF^{+} \rangle}{(E_{AF^{+}} - E_{m})(E_{AF^{+}} - E_{k})} - \langle AF^{+} | H_{x} | AF^{+} \rangle \sum_{m} \frac{|\langle AF^{+} | H_{x} | m \rangle|^{2}}{(E_{AF^{+}} - E_{m})^{2}}.$$
(29)

First we note that the second term in the above sum vanishes because of (12). Also, when k = m in the above sum, the first sum contains $\langle m | H_x | m \rangle$ which is zero for the same reason. If we now consider terms in the first sum such that $k \neq m$ we have the following situations

$$\langle AF^+ | H_x | m \rangle \neq 0 \Rightarrow S_z(|m\rangle) = \pm 1 \text{ and } \langle k | H_x | AF^+ \rangle \neq 0 \Rightarrow S_z(|k\rangle) = \pm 1.$$
 (30)

If the above set of equations hold, then we have

$$\left|S_{z}(\left|m\right\rangle) - S_{z}(\left|k\right\rangle)\right| = 0 \text{ or } 2 \tag{31}$$

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For the first sum in equation (29) not to vanish, we must have, for every m and k:

$$\langle m | H_x | k \rangle \neq 0.$$
 (32)

This is possible only if (11)

$$\left|S_{z}(\left|m\right\rangle) - S_{z}(\left|k\right\rangle)\right| = 1,$$
(33)

which contradicts equation (31).

We therefore have that

$$E_{AF^+}^{(3)} = 0. (34)$$

In fact, it is clear there can be no odd-order contributions to the energy corrections due to the following reason. The lead sum in *m* th order perturbation has a product of *m* matrix elements in the numerator for any combination of the summation indices. If *m* is odd, then if the first (m-1)/2 matrix elements, as well as the last (m-1)/2 matrix elements are non-vanishing, then the remaining matrix element (in the (m+1)/2 position) has the form $\langle r | H_x | s \rangle$ such that

$$S_z(|r\rangle) = \pm S_z(|s\rangle) = \pm \frac{m-1}{2}.$$
(35)

This matrix element $\langle r | H_x | s \rangle$ will therefore be zero by virtue of (2.1.1).

The remaining terms in the expression for the mth order correction to the energy will be proportional to odd order correction terms and hence will vanish on account of this present argument.

2.1.4 Fourth order correction

The fourth order correction to the antiferromagnetic energy is given by

$$E_{AF^{+}}^{(4)} = \sum_{ijk} \frac{\left\langle AF^{+} \left| H_{x} \right| i \right\rangle \left\langle i \left| H_{x} \right| j \right\rangle \left\langle j \left| H_{x} \right| k \right\rangle \left\langle k \left| H_{x} \right| AF^{+} \right\rangle}{(E_{AF^{+}}^{(0)} - E_{i}^{(0)})(E_{AF^{+}}^{(0)} - E_{j}^{(0)})(E_{AF^{+}}^{(0)} - E_{k}^{(0)})} - E_{AF^{+}}^{(2)} \sum_{k} \frac{\left\langle AF^{+} \left| H_{x} \right| k \right\rangle \left\langle k \left| H_{x} \right| AF^{+} \right\rangle}{(E_{AF^{+}}^{(0)} - E_{k}^{(0)})^{2}}.$$
(36)

If $\{a_r\}, r = 1, 2, ..., N\}$ be the set of states with non-vanishing matrix element with $|AF^+\rangle$, that is, such that

$$\left\langle AF^{+}\left|H_{x}\right|a_{r}\right
angle \neq0,$$
(37)

then the expression for $E_{AF^+}^{(4)}$ simplifies to

$$E_{AF^{+}}^{(4)} = \sum_{rs} \left(\frac{\langle AF^{+} | H_{x} | a_{r} \rangle \langle a_{s} | H_{x} | AF^{+} \rangle}{(E_{AF^{+}}^{(0)} - E_{a_{r}}^{(0)})(E_{AF^{+}}^{(0)} - E_{a_{s}}^{(0)})} \sum_{j} \frac{\langle a_{r} | H_{x} | j \rangle \langle j | H_{x} | a_{s} \rangle}{E_{AF^{+}}^{(0)} - E_{j}^{(0)}} \right) - E_{AF^{+}}^{(2)} \sum_{r} \frac{\left| \langle AF^{+} | H_{x} | a_{r} \rangle \right|^{2}}{(E_{AF^{+}}^{(0)} - E_{a_{r}}^{(0)})^{2}}.$$
(38)

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A Maple procedure was written to evaluate the above sums. The first sum evaluates to

$$\sum_{r_{s}} \left\{ \frac{\langle AF^{+} | H_{x} | a_{r} \rangle \langle a_{s} | H_{x} | AF^{+} \rangle}{(E_{\alpha_{F}^{+}}^{(0)} - E_{a_{r}}^{(0)})(E_{\alpha_{F}^{+}}^{(0)} - E_{a_{s}}^{(0)})} \sum_{j} \frac{\langle a_{r} | H_{x} | j \rangle \langle j | H_{x} | a_{s} \rangle}{E_{\alpha_{F}^{+}}^{(0)} - E_{j}^{(0)}} \right) = \frac{Nh_{x}^{4}}{32} \frac{1}{(-1+j-\alpha-h_{z})^{2}} \left\{ \frac{2}{-1+2j-2\alpha} + \frac{N/4-1}{-1+j-\alpha} + \frac{N/4-3/2}{-1+j-h_{z}-\alpha} + \frac{2}{-2+j-2\alpha-2h_{z}} \right\} + \frac{Nh_{x}^{4}}{32} \frac{1}{(-1+j-\alpha+h_{z})^{2}} \left\{ \frac{2}{-1+2j-2\alpha} + \frac{N/4-1}{-1+j-\alpha} + \frac{N/4-3/2}{-1+j-h_{z}-\alpha} + \frac{2}{-2+j-2\alpha-2h_{z}} \right\} + \frac{Nh_{x}^{4}}{16} \left\{ \frac{1}{(-1+j-\alpha+h_{z})^{2}(-2+j-2\alpha+2h_{z})} + \frac{1}{(-1+j-\alpha-h_{z})^{2}(-2+j-2\alpha-2h_{z})} \right\} + \frac{N(N-6)h_{x}^{4}}{128} \left\{ \frac{1}{(-1+j-\alpha+h_{z})^{3}} + \frac{1}{(-1+j-\alpha-h_{z})^{2}(-2+j-2\alpha-2h_{z})} \right\} + \frac{Nh_{x}^{4}}{16} \frac{1}{(-1+j-\alpha-h_{z})(-1+j-\alpha+h_{z})} \left\{ \frac{N/4-1}{-1+j-\alpha} + \frac{2}{-1+2j-2\alpha} \right\},$$
(39)

while the second sum yields

$$-E_{AF^{+}}^{(2)}\sum_{r}\frac{\left|\left\langle AF^{+}\left|H_{x}\right|a_{r}\right\rangle\right|^{2}}{\left(E_{AF^{+}}^{(0)}-E_{r}^{(0)}\right)^{2}}$$

$$=-\frac{N^{2}h_{x}^{4}}{64}\left(\frac{1}{\left(-1+j-\alpha+h_{z}\right)^{2}}+\frac{1}{\left(-1+j-\alpha-h_{z}\right)^{2}}\right)\left(\frac{1}{\left(-1+j-\alpha+h_{z}\right)}+\frac{1}{\left(-1+j-\alpha-h_{z}\right)}\right).$$
(40)

Substituting (39) and (40) for the sums in equation (38), and noting that the terms proportional to N^2 cancel out, we have

$$\begin{split} E_{AF^{+}}^{(4)} &= \frac{Nh_{x}^{4}}{32} \frac{1}{(-1+j-\alpha-h_{z})^{2}} \Biggl\{ \frac{2}{-1+2j-2\alpha} + \frac{1}{1-j+\alpha} + \frac{3/2}{1-j+h_{z}+\alpha} - \frac{2}{2-j+2\alpha+2h_{z}} \Biggr\} \\ &+ \frac{Nh_{x}^{4}}{32} \frac{1}{(-1+j-\alpha+h_{z})^{2}} \Biggl\{ \frac{2}{-1+2j-2\alpha} + \frac{1}{1-j+\alpha} + \frac{3/2}{1-j-h_{z}+\alpha} - \frac{2}{2-j+2\alpha-2h_{z}} \Biggr\} \\ &- \frac{Nh_{x}^{4}}{16} \frac{1}{(-1+j-\alpha-h_{z})(-1+j-\alpha+h_{z})} \Biggl\{ \frac{1}{-1+j-\alpha} - \frac{2}{-1+2j-2\alpha} \Biggr\} \\ &+ \frac{Nh_{x}^{4}}{16} \Biggl\{ \frac{1}{(-1+j-\alpha+h_{z})^{2}(-2+j-2\alpha+2h_{z})} + \frac{1}{(-1+j-\alpha-h_{z})^{2}(-2+j-2\alpha-2h_{z})} \Biggr\} \end{split}$$

.

$$-\frac{3Nh_{x}^{4}}{64}\left\{\frac{1}{\left(-1+j-\alpha+h_{z}\right)^{3}}+\frac{1}{\left(-1+j-\alpha-h_{z}\right)^{3}}\right\}.$$
(41)

Substituting $\alpha = 0$ in (41) and dividing by N, we find the fourth order correction to the antiferromagnetic ground state energy per spin to be

$$\varepsilon_{AF^{+}}^{(4)} = \frac{h_{x}^{4}}{32} \frac{1}{(-1+j-h_{z})^{2}} \left\{ \frac{2}{-1+2j} + \frac{1}{1-j} + \frac{3/2}{1-j+h_{z}} - \frac{2}{2-j+2h_{z}} \right\}$$

$$+ \frac{h_{x}^{4}}{32} \frac{1}{(-1+j+h_{z})^{2}} \left\{ \frac{2}{-1+2j} + \frac{1}{1-j} + \frac{3/2}{1-j-h_{z}} - \frac{2}{2-j-2h_{z}} \right\}$$

$$- \frac{h_{x}^{4}}{16} \frac{1}{(-1+j-h_{z})(-1+j+h_{z})} \left\{ \frac{1}{-1+j} - \frac{2}{-1+2j} \right\}$$

$$+ \frac{h_{x}^{4}}{16} \left\{ \frac{1}{(-1+j+h_{z})^{2}(-2+j+2h_{z})} + \frac{1}{(-1+j-h_{z})^{2}(-2+j-2h_{z})} \right\}$$

$$- \frac{3h_{x}^{4}}{64} \left\{ \frac{1}{(-1+j+h_{z})^{3}} + \frac{1}{(-1+j-h_{z})^{3}} \right\}.$$

$$(42)$$

From equations (9), (19) and (42), we have

$$\mathcal{E}_{AF^{+}}(\alpha, j, h_{x}, h_{z}) = -\frac{(1-j+2\alpha)}{4} - \frac{h_{x}^{2}}{8} \left\{ \frac{1}{1-j+\alpha+h_{z}} + \frac{1}{1-j+\alpha-h_{z}} \right\}$$

$$+ \frac{h_{x}^{4}}{32} \frac{1}{(-1+j-\alpha-h_{z})^{2}} \left\{ \frac{2}{-1+2j-2\alpha} + \frac{1}{1-j+\alpha} + \frac{3/2}{1-j+h_{z}+\alpha} - \frac{2}{2-j+2\alpha+2h_{z}} \right\}$$

$$+ \frac{h_{x}^{4}}{32} \frac{1}{(-1+j-\alpha+h_{z})^{2}} \left\{ \frac{2}{-1+2j-2\alpha} + \frac{1}{1-j+\alpha} + \frac{3/2}{1-j-h_{z}+\alpha} - \frac{2}{2-j+2\alpha-2h_{z}} \right\}$$

$$- \frac{h_{x}^{4}}{16} \frac{1}{(-1+j-\alpha-h_{z})(-1+j-\alpha+h_{z})} \left\{ \frac{1}{-1+j-\alpha} - \frac{2}{-1+2j-2\alpha} \right\}$$

$$+ \frac{h_{x}^{4}}{16} \left\{ \frac{1}{(-1+j-\alpha+h_{z})^{2}(-2+j-2\alpha+2h_{z})} + \frac{1}{(-1+j-\alpha-h_{z})^{2}(-2+j-2\alpha-2h_{z})} \right\}$$

$$- \frac{3h_{x}^{4}}{64} \left\{ \frac{1}{(-1+j-\alpha+h_{z})^{3}} + \frac{1}{(-1+j-\alpha-h_{z})^{3}} \right\}.$$

$$(43)$$

The antiferromagnetic ground state energy per spin, to the fourth order in h_x is therefore given by

$$\begin{split} & \varepsilon_{AF^{+}}(0,j,h_{x},h_{z}) = -\frac{(1-j)}{4} - \frac{h_{x}^{2}}{8} \Biggl\{ \frac{1}{1-j+h_{z}} + \frac{1}{1-j-h_{z}} \Biggr\} \\ & + \frac{h_{x}^{4}}{32} \frac{1}{(-1+j-h_{z})^{2}} \Biggl\{ \frac{2}{-1+2j} + \frac{1}{1-j} + \frac{3/2}{1-j+h_{z}} - \frac{2}{2-j+2h_{z}} \Biggr\} \\ & + \frac{h_{x}^{4}}{32} \frac{1}{(-1+j+h_{z})^{2}} \Biggl\{ \frac{2}{-1+2j} + \frac{1}{1-j} + \frac{3/2}{1-j-h_{z}} - \frac{2}{2-j-2h_{z}} \Biggr\} \end{split}$$

$$-\frac{h_{x}^{4}}{16}\frac{1}{(-1+j-h_{z})(-1+j+h_{z})}\left\{\frac{1}{-1+j}-\frac{2}{-1+2j}\right\}$$
$$+\frac{h_{x}^{4}}{16}\left\{\frac{1}{(-1+j+h_{z})^{2}(-2+j+2h_{z})}+\frac{1}{(-1+j-h_{z})^{2}(-2+j-2h_{z})}\right\}$$
$$-\frac{3h_{x}^{4}}{64}\left\{\frac{1}{(-1+j+h_{z})^{3}}+\frac{1}{(-1+j-h_{z})^{3}}\right\}.$$
(44)

The simplest case of equation (44) is the transverse Ising model, $h_z = 0 = j$, and the ground state energy per spin is

$$\mathcal{E}_{AF^+} = -\frac{1}{4} - \frac{h_x^2}{4} - \frac{h_x^4}{16}.$$
(45)

The exact ground state energy per spin of the transverse Ising model is [7, 8, 9]

$$\frac{E_0}{N} = -\frac{(1+2h_x)}{2\pi} \mathsf{E}\left(\frac{\sqrt{8h_x}}{(1+2h_x)}\right)$$
$$= -\frac{1}{4} - \frac{h_x^2}{4} - \frac{h_x^4}{16} + \mathcal{O}(h_x^6).$$
(46)

Thus we see that the perturbation expansion (45) gives the correct energy per spin for the Ising model in a transverse field to the fourth order in h_x .

3 The ferromagnetic ground state

The ground state of the longitudinal ANNNI model (1) is the non-degenerate all-spin up ferromagnetic state in the region bounded by the h_z axis and the line $h_z = 1 + j$ in the $h_z - j$ plane. That is, the unperturbed ground state is

$$|F\rangle = |\uparrow\uparrow\uparrow\uparrow\uparrow\cdots\uparrow\uparrow\rangle,\tag{47}$$

with corresponding energy

$$E_F^{(0)} = \frac{N(1+j)}{4} - \frac{Nh_z}{2}.$$
(48)

We note that the ground state is ferromagnetic only for finite h_z , this is in contrast to the situation in a ferromagnetic model. The inversion symmetry which makes the all-spin up and all-spin down state to be degenerate is removed by the presence of a finite longitudinal field, h_z , so that the ground state is the all-spin up nondegenerate state in the indicated region. The longitudinal field h_z however does not break the translational invariance symmetry of the Hamiltonian. We see also that the presence of h_z makes the Hamiltonian to already be in a form where can apply the Feynman technique directly to calculate the various physical quantities. We recall

$$H = H_z + H_x, \tag{49}$$

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where

$$H_{z} = \sum_{i} S_{i}^{z} S_{i+1}^{z} + \sum_{i} S_{i}^{z} S_{i+2}^{z} - h_{z} \sum_{i} S_{i}^{z}$$
(50)

$$H_x = -h_x \sum_i S_i^x \,. \tag{51}$$

3.1 Energy corrections

The first order correction $E_F^{(0)}$ to the ferromagnetic ground state energy is

$$E_F^{(0)} = \left\langle F \left| H_x \right| F \right\rangle. \tag{52}$$

This quantity vanishes, on account of equation (12).

3.1.1 Second order correction

The second order correction to the ground state energy is given by

$$E_{F}^{(2)} = \sum_{j} \frac{\langle F | H_{x} | j \rangle \langle j | H_{x} | F \rangle}{E_{F}^{(0)} - E_{j}^{(0)}}$$
$$= \sum_{j} \frac{\left| \langle F | H_{x} | j \rangle \right|^{2}}{E_{F}^{(0)} - E_{j}^{(0)}}.$$
(53)

The only non-vanishing matrix elements in the above sum are those contributed by the N-fold degenerate N-1 spins up, 1 spin down states, $|m\rangle$, any linear combination of which is also a first excited state of the ferromagnetic ground state. The degenerate unperturbed energy of $|m\rangle$ is

$$E_{|m\rangle}^{(0)} = \left(\frac{N}{4} - 1\right) (1+j) - \left(\frac{N}{2} - 1\right) h_z,$$
(54)

with

$$m\rangle \in \left\{\uparrow\uparrow\uparrow\uparrow\uparrow\cdots\uparrow\downarrow\rangle, |\uparrow\uparrow\uparrow\cdots\uparrow\downarrow\uparrow\rangle, \cdots, |\downarrow\uparrow\uparrow\uparrow\cdots\uparrow\uparrow\rangle\right\}.$$
(55)

We therefore have from equation (48) and (54) that the energy shift is

$$E_F^{(0)} - E_m^{(0)} = 1 + j - h_z . ag{56}$$

The second order correction to the ferromagnetic ground state energy is therefore

$$E_F^{(2)} = \frac{Nh_x^2}{4} \frac{1}{(1+j-h_z)}.$$
(57)

We remark that perturbation expansions with terms similar to that in equation (57) have been obtained in a quantum modelling of the two-dimensional ANNNI model by Barber and Duxbury [10], for a ferromagnetic model. The said paper was not concerned with the longitudinal ANNNI model and in fact the longitudinal field was introduced merely as an artifice to enable the calculation of the ferromagnetic order parameter and the associated susceptibility.

With argument similar to that in the previous section, we find that the third order correction to the ferromagnetic ground state energy vanishes.

Next we will compute the fourth-order correction to the ferromagnetic ground state energy.

3.1.2 Fourth order correction

The fourth-order correction to the ground state energy is given by

$$E_{F}^{(4)} = \sum_{ijk} \frac{\langle F | H_{x} | i \rangle \langle i | H_{x} | j \rangle \langle j | H_{x} | k \rangle \langle k | H_{x} | F \rangle}{(E_{F}^{(0)} - E_{i}^{(0)})(E_{F}^{(0)} - E_{j}^{(0)})(E_{F}^{(0)} - E_{k}^{(0)})} - E_{F}^{(2)} \sum_{k} \frac{\langle F | H_{x} | k \rangle \langle k | H_{x} | F \rangle}{(E_{F}^{(0)} - E_{k}^{(0)})^{2}}.$$
(58)

If $\{|a_r\rangle, r = 1, 2, ..., N\}$ (equivalent to the set $\{|m\rangle\}$ of equation (55)) be the set of states with non-vanishing matrix element with $|F\rangle$, that is, such that

$$\left\langle F\left|H_{x}\right|a_{r}\right\rangle \neq0,\tag{59}$$

then the expression for $E_F^{(4)}$ simplifies to

$$E_{F}^{(4)} = \sum_{rs} \left(\frac{\langle F | H_{x} | a_{r} \rangle \langle a_{s} | H_{x} | F \rangle}{(E_{F}^{(0)} - E_{a_{r}}^{(0)})(E_{F}^{(0)} - E_{a_{s}}^{(0)})} \sum_{j} \frac{\langle a_{r} | H_{x} | j \rangle \langle j | H_{x} | a_{s} \rangle}{E_{F}^{(0)} - E_{j}^{(0)}} \right) - E_{F}^{(2)} \sum_{r} \frac{\left| \langle F | H_{x} | a_{r} \rangle \right|^{2}}{(E_{F}^{(0)} - E_{a_{r}}^{(0)})^{2}}.$$
(60)

A Maple procedure computes $E_F^{(4)}$ as

$$E_{F}^{(4)} = \frac{Nh_{x}^{4}}{16(1+j-h_{z})^{2}} \left(\frac{2}{1+2j-2h_{z}} + \frac{2}{2+j-2h_{z}} + \frac{(N-5)/2}{1+j-h_{z}} \right) + \frac{Nh_{x}^{4}}{8(1+j-h_{z})^{2}} \left(\frac{1}{(1+2j-2h_{z})} + \frac{1}{2+j-2h_{z}} \right) + \frac{h_{x}^{4}N(N-5)}{32(1+j-h_{z})^{3}} - \frac{N^{2}h_{x}^{4}}{16(1+j-h_{z})^{3}}.$$
(61)

We observe that the terms proportional to N^2 cancel out and we are left with

$$E_F^{(4)} = \frac{Nh_x^4}{16(1+j-h_z)^2} \left(\frac{-5}{(1+j-h_z)} + \frac{4}{(2+j-2h_z)} + \frac{4}{(1+2j-2h_z)}\right).$$
 (62)

The expression (62) is always positive. This is easy to see when we recall that the ground state of the longitudinal ANNNI model is ferromagnetic for $h_z > j+1$. Substitution of $h_z = j+1+\delta$ in (62) (δ a positive quantity) gives

$$E_F^{(4)} = \frac{Nh_x^4}{16\delta^2} \left(\frac{5j + 6\delta + 6j\delta + 4\delta^2}{\delta(j + 2\delta)(1 + 2\delta)} \right),\tag{63}$$

which is clearly a positive quantity.

Combining equations (48), (57) and (62), we therefore have that to fourth-order in the transverse field h_x , the ferromagnetic ground state energy of the ANNNI model in mixed field is given by

$$E_{F} = \frac{Nh_{x}^{4}}{16(1+j-h_{z})^{2}} \left(\frac{-5}{(1+j-h_{z})} + \frac{4}{(2+j-2h_{z})} + \frac{4}{(1+2j-2h_{z})} \right) + \frac{Nh_{x}^{2}}{4(1+j-h_{z})} + \frac{N(1+j-2h_{z})}{4}.$$
(64)

3.2 Physical quantities

Having obtained the approximate ferromagnetic ground state energy, we are now in a position to calculate various quantities of physical interest, the ferromagnetic order parameter, the magnetic susceptibility and the specific heat. The form of the Hamiltonian makes it easy to compute these quantities using Feynman's theorem [11]

3.2.1 Ferromagnetic order parameter

Using Feynman's theorem

$$\left\langle F \left| \frac{\partial H}{\partial h_z} \right| F \right\rangle = \frac{\partial E_F}{\partial h_z},$$
(65)

the ferromagnetic order parameter of the ANNNI model in mixed fields is given by

$$\eta_{F} = 2 < \sum_{i} S_{i}^{z} > /N$$

$$= -2/N\partial E_{F}/\partial h_{z}$$

$$= -2\partial \varepsilon_{F}/\partial h_{z}$$

$$= 1 - \frac{1}{2} \frac{h_{x}^{2}}{(1+j-h_{z})^{2}} - \frac{1}{4} \frac{h_{x}^{4}}{(1+j-h_{z})^{3}} \left(\frac{-5}{1+j-h_{z}} + \frac{4}{2+j-2h_{z}} + \frac{4}{1+2j-2h_{z}} \right)$$

$$- \frac{1}{8} \frac{h_{x}^{4}}{(1+j-h_{z})^{2}} \left(\frac{-5}{(1+j-h_{z})^{2}} + \frac{8}{(2+j-2h_{z})^{2}} + \frac{8}{(1+2j-2h_{z})^{2}} \right). \quad (66)$$

The susceptibility is given by $2^2 - 2t^2$

$$\chi_{F} = \partial^{2} \varepsilon_{F} / \partial h_{z}^{2}$$

$$= -\frac{h_{x}^{2}}{(1+j-h_{z})^{3}} - \frac{3}{4} \frac{h_{x}^{4}}{(1+j-h_{z})^{4}} \left(\frac{-5}{1+j-h_{z}} + \frac{4}{2+j-2h_{z}} + \frac{4}{1+2j-2h_{z}} \right)$$

$$-\frac{1}{2} \frac{h_{x}^{4}}{(1+j-h_{z})^{3}} \left(\frac{-5}{(1+j-h_{z})^{2}} + \frac{8}{(2+j-2h_{z})^{2}} + \frac{8}{(1+2j-2h_{z})^{2}} \right)$$

$$-\frac{1}{4} \frac{h_{x}^{4}}{(1+j-h_{z})^{2}} \left(\frac{-5}{(1+j-h_{z})^{3}} + \frac{16}{(2+j-2h_{z})^{3}} + \frac{16}{(1+2j-2h_{z})^{3}} \right).$$
(67)

3.2.2 Specific Heat

The specific heat of the ferromagnetic ground state ANNNI model in mixed fields is given by

$$c = -\frac{1}{N} \frac{d^2 E_0}{dh_x^2}$$

= $-\frac{1}{2} \frac{1}{1+j-h_z} - \frac{3}{4} \frac{h_x^2}{(1+j-h_z)^2} \left(\frac{-5}{1+j-h_z} + \frac{4}{2+j-2h_z} + \frac{4}{1+2j-2h_z} \right).$ (68)

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4 The antiphase ground state

The ground state of the longitudinal ANNNI model (1) in the region bounded by the line $2h_z + 1 = 2j$ and the j axis is the four-fold degenerate antiphase states, with two spins up followed by two spins down. Classified by translational invariance, the states occur in the subspaces k = 0, k = N/4, k = N/2 and k = 3N/4 of the eigenstates of T (one linear combination in each subspace). In order to simulate the antiphase states correctly, we will assume that N is a multiple of 4. The degenerate energy is

$$E_{<2>}^{(0)} = -\frac{Nj}{4},\tag{69}$$

belonging to each of the 4 states

$$\begin{split} |\langle 2 \rangle \rangle_{a} &= \left| \uparrow \uparrow \downarrow \downarrow \cdots \uparrow \uparrow \downarrow \downarrow \right\rangle, \\ |\langle 2 \rangle \rangle_{b} &= \left| \uparrow \downarrow \downarrow \uparrow \cdots \uparrow \downarrow \downarrow \uparrow \right\rangle, \\ |\langle 2 \rangle \rangle_{c} &= \left| \downarrow \downarrow \uparrow \uparrow \cdots \downarrow \downarrow \uparrow \uparrow \right\rangle, \\ and |\langle 2 \rangle \rangle_{d} &= \left| \downarrow \uparrow \uparrow \downarrow \cdots \downarrow \uparrow \uparrow \downarrow \right\rangle. \end{split}$$

$$(70)$$

In order to facilitate the calculation of the order parameter and the susceptibility, we introduce in the unperturbed Hamiltonian (1), a field, $\beta > 0$, and write the unperturbed Hamiltonian as

$$H_{z} = \sum_{i=1}^{N} S_{i}^{z} S_{i+1}^{z} + \sum_{i=1}^{N} S_{i}^{z} S_{i+2}^{z} - h_{z} \sum_{i=1}^{N} S_{i}^{z} - \beta \sum_{k=1}^{N/4} \left(S_{4k-3}^{z} + S_{4k-2}^{z} - S_{4k-1}^{z} - S_{4k}^{z} \right).$$
(71)

This way, the antiphase order parameter, $\rho_{<2>}$, and the associated susceptibility, $\chi_{<2>}$ can be calculated from

$$\rho = -\frac{2}{N} \frac{\partial E_{<2>}}{\partial \beta} \bigg|_{\beta=0}$$

and $\chi = -\frac{2}{N} \frac{\partial^2 E_{<2>}}{\partial \beta^2} \bigg|_{\beta=0}$. (72)

We note that the field β breaks the translational invariance symmetry of the Hamiltonian *H*. A finite β also lifts the degeneracy of the antiphase states, although not completely. $|\langle 2 \rangle\rangle_{b}$ and $|\langle 2 \rangle\rangle_{d}$ are not sensitive to the field β , and so they remain degenerate, with the energy remaining the same as in (69), while $|\langle 2 \rangle\rangle_{a}$ and $|\langle 2 \rangle\rangle_{c}$ now have energies given by

$$E_{<2>_a}^{(0)} = -\frac{N(j+2\beta)}{4} \operatorname{and} E_{<2>_c}^{(0)} = -\frac{N(j-2\beta)}{4}.$$
(73)

We see that $|\langle 2 \rangle\rangle_a$ is the non-degenerate ground state of the unperturbed Hamiltonian (1) in the region between the *j* axis and the line $2h_z + 1 = 2j$, for a finite β .

4.1 Energy corrections

4.1.1 First order correction

In zero field β , the ground state of Hamiltonian (71) is four-fold degenerate, so that the 4×4 perturbation matrix V, has elements

$$V_{ij} = \left\langle <2 >_i \left| H_x \right| <2 >_j \right\rangle.$$
(74)

where the states $|\langle 2\rangle_s \rangle$ are given in (70). All sixteen elements of V vanish on account of (12), so that as in the previous cases, the first order correction to the ground state energy of the antiphase states is zero.

4.1.2 Second order correction

The perturbation matrix for the second order correction to the antiphase ground state energy has elements

$$V_{ij} = \sum_{m} \frac{\langle \langle 2 \rangle_{i} | H_{x} | m \rangle \langle m | H_{x} | \langle 2 \rangle_{j} \rangle}{E_{\langle 2 \rangle}^{(0)} - E_{m}^{(0)}}.$$
(75)

It is clear that it is impossible to have a state $|m\rangle$ in the 2^N dimensional Hilbert space of the Hamiltonian of N spins simultaneously having nonzero matrix element with two different members of the four-fold degenerate $|\langle 2 \rangle\rangle$ states. In other words, the matrix V is diagonal, with

$$V_{ii} = \sum_{m} \frac{\left| \left\langle <2 >_{i} \left| H_{x} \right| m \right\rangle \right|^{2}}{E_{<2>_{i}}^{(0)} - E_{m}^{(0)}},$$
(76)

which are just the Rayleigh-Schrödinger expressions for second-order corrections to the energy in non-degenerate perturbation theory.

Putting i = a, b, c, d in turns in (76), we have

$$E_{<2>_{a}}^{(2)} = -\frac{Nh_{x}^{2}}{8} \left(\frac{1}{j+h_{z}+\beta} + \frac{1}{j-h_{z}+\beta} \right),$$
(77)

$$E_{<2>_{b}}^{(2)} = -\frac{Nh_{x}^{2}}{16} \left(\frac{1}{j+h_{z}+\beta} + \frac{1}{j-h_{z}-\beta} + \frac{1}{j-h_{z}+\beta} + \frac{1}{j+h_{z}-\beta} \right) = E_{<2>_{d}}^{(0)}$$
(78)

and

$$E_{<2>_{c}}^{(2)} = -\frac{Nh_{x}^{2}}{8} \left(\frac{1}{j+h_{z}-\beta} + \frac{1}{j-h_{z}-\beta} \right).$$
(79)

Equations (77), (78) and (79) contain an interesting summary of the properties of the general Hamiltonian *H* of the ANNNI model in mixed fields. We note that although the introduction of the field β breaks the translational invariance symmetry of the Hamiltonian, it does leave the reflection symmetry intact. In fact every eigenstate of the reflection operator R is also an eigenstate of the operator $\beta \sum_{i=1}^{N/4} (S_{4k-3}^z + S_{4k-2}^z - S_{4k-1}^z - S_{4k}^z)$ with eigenvalue 0. That is, for any

 $|\psi\rangle$ an eigenstate of total S_z , we have

$$\left(\beta \sum_{i=1}^{N/4} \left(S_{4k-3}^{z} + S_{4k-2}^{z} - S_{4k-1}^{z} - S_{4k}^{z} \right) \right) \psi \rangle = 0,$$
(80)

whenever

$$\mathsf{R}|\psi\rangle = \pm|\psi\rangle. \tag{81}$$

In other words, eigenstates of R do not sense the presence of the field β .

Each of the two states (and hence their linear combination)

$$|\langle 2 \rangle\rangle_{b} = |\uparrow\downarrow\downarrow\uparrow\uparrow\cdots\uparrow\downarrow\downarrow\uparrow\rangle$$
 and $|\langle 2 \rangle\rangle_{d} = |\downarrow\uparrow\uparrow\downarrow\cdots\downarrow\uparrow\uparrow\downarrow\rangle$ (82)

is an eigenstate of R. This explains their degeneracy at zeroth-order perturbation and why the second order energy corrections in these states are the same. Since [H,R]=0, it is expected that their degeneracy will not be lifted, to any order in perturbation. It is also noteworthy that $|\langle 2 \rangle\rangle_b$ and $|\langle 2 \rangle\rangle_d$ are related by the inversion symmetry, which however is not a symmetry of H for finite h_z .

As for

$$|\langle 2 \rangle\rangle_{a} = |\uparrow\uparrow\downarrow\downarrow\downarrow\cdots\uparrow\uparrow\downarrow\downarrow\rangle$$
 and $|\langle 2 \rangle\rangle_{c} = |\downarrow\downarrow\uparrow\uparrow\uparrow\cdots\downarrow\downarrow\uparrow\uparrow\rangle$ (83)

the translational invariance which connects the two states is removed by the field β and they cease to be degenerate. We observe also that the two states are related by the inversion symmetry, but this is not a symmetry of the Hamiltonian, except at $h_z = 0$ (corresponding to the ANNNI model in a transverse field). Results for one state can be obtained from the other by replacing β in one with $-\beta$ in the other.

Putting $\beta = 0$ in (77), (78) and (79) we see that the degeneracy in the antiphase states remain to second order in perturbation in h_{y} .

4.1.3 Fourth order correction

For simplicity we will drop the subscript *a* on $|\langle 2\rangle_a\rangle$ henceforth and simply refer to the antiphase ground state by $|\langle 2\rangle\rangle$. The fourth-order correction to the ground state energy of the antiphase ground state is given by

$$E_{<2>}^{(4)} = \sum_{ijk} \frac{\langle <2 > |H_x|i\rangle\langle i|H_x|j\rangle\langle j|H_x| <2 >\rangle}{(E_{<2>}^{(0)} - E_i^{(0)})(E_{<2>}^{(0)} - E_j^{(0)})(E_{<2>}^{(0)} - E_k^{(0)})} - E_{<2>}^{(2)} \sum_k \frac{\langle <2 > |H_x|k\rangle\langle k|H_x| <2 >\rangle}{(E_{<2>}^{(0)} - E_k^{(0)})^2}.$$
(84)

If $\{|a_r\rangle\}$, $r = 1, 2, \dots, N$ denotes the set of states with non-vanishing matrix elements with $|\langle 2 \rangle\rangle$, then the above expression simplifies to

$$E_{<2>}^{(4)} = \sum_{rs} \left(\frac{\langle <2> |H_x|a_r \rangle \langle a_r |H_x|<2> \rangle}{(E_{<2>}^{(0)} - E_{a_r}^{(0)})(E_{<2>}^{(0)} - E_{a_s}^{(0)})} \sum_j \frac{\langle a_r |H_x|j \rangle \langle j |H_x|a_s \rangle}{E_{<2>}^{(0)} - E_j^{(0)}} \right) - E_{<2>}^{(2)} \sum_r \frac{\left| \langle <2> |H_x|a_r \rangle \right|^2}{(E_{<2>}^{(0)} - E_{a_r}^{(0)})^2}.$$
(85)

A Maple procedure evaluates the above sum to

$$E_{<2>}^{(4)} = -\frac{Nh_x^4}{32} \frac{1}{(j+\beta+h_z)^2} \left(\frac{1}{2j+2\beta+1+2h_z} + \frac{2}{j+2\beta} + \frac{1}{2j+2\beta-1} + \frac{N/4-1}{j+\beta+h_z} + \frac{N/4-3/2}{j+\beta} \right)$$

$$-\frac{Nh_{x}^{4}}{32}\frac{1}{(j+\beta-h_{z})^{2}}\left(\frac{1}{2j+2\beta+1-2h_{z}}+\frac{2}{j+2\beta}+\frac{1}{2j+2\beta-1}+\frac{N/4-1}{j+\beta-h_{z}}+\frac{N/4-3/2}{j+\beta}\right)$$
$$-\frac{Nh_{x}^{4}}{32}\left(\frac{1}{(j+\beta+h_{z})^{2}(2j+2\beta+1+2h_{z})}+\frac{1}{(j+\beta-h_{z})^{2}(2j+2\beta+1-2h_{z})}\right)$$
$$-\frac{Nh_{x}^{4}}{32}\frac{1}{(j+\beta+h_{z})(j+\beta-h_{z})}\left(\frac{2}{2j+2\beta-1}+\frac{(N/2-3)}{j+\beta}+\frac{4}{j+2\beta}\right)$$
$$-\frac{Nh_{x}^{4}}{32}\left(\frac{N}{4}-1\right)\left(\frac{1}{(j+\beta+h_{z})^{3}}+\frac{1}{(j+\beta-h_{z})^{3}}\right)$$
$$+\frac{Nh_{x}^{4}}{64}\left(\frac{1}{(j+\beta+h_{z})^{2}}+\frac{1}{(j+\beta-h_{z})^{2}}\right)\left(\frac{1}{(j+\beta+h_{z})}+\frac{1}{(j+\beta-h_{z})}\right).$$
(86)

If we denote the terms proportional to N^2 in the above equation by s_{N^2} , then

$$s_{N^{2}} = -\frac{N^{2}h_{x}^{4}}{64} \frac{1}{(j+\beta+h_{z})^{3}} - \frac{N^{2}h_{x}^{4}}{128} \frac{1}{(j+\beta+h_{z})^{2}} \frac{1}{j+\beta}$$

$$-\frac{N^{2}h_{x}^{4}}{64} \frac{1}{(j+\beta-h_{z})^{3}} - \frac{N^{2}h_{x}^{4}}{128} \frac{1}{(j+\beta-h_{z})^{2}} \frac{1}{j+\beta}$$

$$-\frac{N^{2}h_{x}^{4}}{64} \frac{1}{(j+\beta+h_{z})(j+\beta-h_{z})(j+\beta)}$$

$$+\frac{N^{2}h_{x}^{4}}{64} \frac{1}{(j+\beta+h_{z})^{3}} + \frac{N^{2}h_{x}^{4}}{64} \frac{1}{(j+\beta+h_{z})^{2}} \frac{1}{(j+\beta-h_{z})}$$

$$+\frac{N^{2}h_{x}^{4}}{64} \frac{1}{(j+\beta-h_{z})^{2}} \frac{1}{(j+\beta+h_{z})} + \frac{N^{2}h_{x}^{4}}{64} \frac{1}{(j+\beta-h_{z})^{3}}$$

$$= 0.$$
(87)

We therefore have that the fourth order correction to the antiphase ground state is given by

$$E_{<2>}^{(4)} = -\frac{Nh_x^4}{32} \frac{1}{(j+\beta+h_z)^2} \left(\frac{1}{2j+2\beta+1+2h_z} + \frac{2}{j+2\beta} + \frac{1}{2j+2\beta-1} - \frac{1}{j+\beta+h_z} - \frac{3/2}{j+\beta} \right)$$

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$$-\frac{Nh_{x}^{4}}{32}\frac{1}{(j+\beta-h_{z})^{2}}\left(\frac{1}{2j+2\beta+1-2h_{z}}+\frac{2}{j+2\beta}+\frac{1}{2j+2\beta-1}-\frac{1}{j+\beta-h_{z}}-\frac{3/2}{j+\beta}\right)$$
$$-\frac{Nh_{x}^{4}}{32}\left(\frac{1}{(j+\beta+h_{z})^{2}(2j+2\beta+1+2h_{z})}+\frac{1}{(j+\beta-h_{z})^{2}(2j+2\beta+1-2h_{z})}\right)$$
$$-\frac{Nh_{x}^{4}}{32}\frac{1}{(j+\beta+h_{z})(j+\beta-h_{z})}\left(\frac{2}{2j+2\beta-1}-\frac{3}{j+\beta}+\frac{4}{j+2\beta}\right)$$
$$+\frac{Nh_{x}^{4}}{32}\left(\frac{1}{(j+\beta+h_{z})^{3}}+\frac{1}{(j+\beta-h_{z})^{3}}\right).$$
(88)

The antiphase ground state energy per spin, to fourth order in the transverse field h_x is therefore given by (equations (73), (77) and (88))

$$\mathcal{E}_{<2>}(\beta=0) = \left\{ -\frac{h_x^4}{32} \frac{1}{(j+\beta+h_z)^2} \left(\frac{1}{2j+2\beta+1+2h_z} + \frac{2}{j+2\beta} + \frac{1}{2j+2\beta-1} - \frac{1}{j+\beta+h_z} - \frac{3/2}{j+\beta} \right) - \frac{h_x^4}{32} \frac{1}{(j+\beta-h_z)^2} \left(\frac{1}{2j+2\beta+1-2h_z} + \frac{2}{j+2\beta} + \frac{1}{2j+2\beta-1} - \frac{1}{j+\beta-h_z} - \frac{3/2}{j+\beta} \right) - \frac{h_x^4}{32} \left(\frac{1}{(j+\beta+h_z)^2(2j+2\beta+1+2h_z)} + \frac{1}{(j+\beta-h_z)^2(2j+2\beta+1-2h_z)} \right) - \frac{h_x^4}{32} \frac{1}{(j+\beta+h_z)(j+\beta-h_z)} \left(\frac{2}{2j+2\beta-1} - \frac{3}{j+\beta} + \frac{4}{j+2\beta} \right) + \frac{h_x^4}{32} \left(\frac{1}{(j+\beta+h_z)^3} + \frac{1}{(j+\beta-h_z)^3} \right) - \frac{h_x^2}{4} \left(\frac{1}{(j+\beta+h_z)} + \frac{1}{(j+\beta-h_z)} \right) - \frac{(j+2\beta)}{4} \right\} \right|_{\beta=0}.$$
(89)

That is

$$\begin{split} \varepsilon_{<2>} &= -\frac{h_x^4}{32} \frac{1}{(j+h_z)^2} \left(\frac{1}{2j+1+2h_z} + \frac{1}{2j} + \frac{1}{2j-1} - \frac{1}{j+h_z} \right) \\ &- \frac{h_x^4}{32} \frac{1}{(j-h_z)^2} \left(\frac{1}{2j+1-2h_z} + \frac{1}{2j} + \frac{1}{2j-1} - \frac{1}{j-h_z} \right) \\ &- \frac{h_x^4}{32} \left(\frac{1}{(j+h_z)^2(2j+1+2h_z)} + \frac{1}{(j-h_z)^2(2j+1-2h_z)} \right) \\ &- \frac{h_x^4}{32} \frac{1}{(j+h_z)(j-h_z)} \left(\frac{2}{2j-1} + \frac{1}{j} \right) \\ &+ \frac{h_x^4}{32} \left(\frac{1}{(j+h_z)^3} + \frac{1}{(j-h_z)^3} \right) \end{split}$$

$$-\frac{h_x^2}{8} \left(\frac{1}{(j+h_z)} + \frac{1}{(j-h_z)} \right) - \frac{j}{4}.$$
 (90)

In particular the ground state energy per spin of the antiphase state for the ANNNI model in a transverse field ($h_z = 0$), to the fourth order in h_x is

$$\varepsilon_{<2>_{tANNNI}} = -\frac{j}{4} - \frac{h_x^2}{4j} - \frac{1}{16j^3} \left(\frac{8j^2}{4j^2 - 1} - 1\right) h_x^4 \,. \tag{91}$$

 $\varepsilon_{<2>_{tANNNI}}$ is always negative since j > 0.5. The ground state energy per spin for the transverse ANNNI model is plotted as a function of h_x in figure 2 for three different values of j.



Figure 2: Transverse field antiphase ANNNI ground state energy per spin as a function of h_x , to the fourth order, for selected values of j.

4.2 Physical quantities of the antiphase ground state **4.2.1** Order parameter

The antiphase long range order parameter is obtained from

$$\begin{split} \rho_{<2>} &= \lim_{N \to \infty} 2 \left\langle \sum_{k=1}^{N4} \left(S_{4k-3}^{z} + S_{4k-2}^{z} + S_{4k-1}^{z} + S_{4k}^{z} \right) \right\rangle / N = -2 \frac{\partial \varepsilon_{<2>}}{\partial \beta} \bigg|_{\beta=0} \\ &= 1 - \frac{h_{x}^{2}}{4} \left(\frac{1}{(j+h_{z})^{2}} + \frac{1}{(j-h_{z})^{2}} \right) \\ &- \frac{1}{8} \frac{h_{x}^{4}}{(j+h_{z})^{3}} \left(\frac{1}{2j+1+2h_{z}} + \frac{1}{2j} + \frac{1}{2j-1} - \frac{1}{j+h_{z}} \right) \\ &- \frac{1}{8} \frac{h_{x}^{4}}{(j-h_{z})^{3}} \left(\frac{1}{2j+1-2h_{z}} + \frac{1}{2j} + \frac{1}{2j-1} - \frac{1}{j-h_{z}} \right) \end{split}$$

$$-\frac{1}{16}\frac{h_x^4}{(j+h_z)^2}\left(\frac{2}{(2j+1+2h_z)^2} + \frac{5}{2j^2} + \frac{2}{(2j-1)^2} - \frac{1}{(j+h_z)^2}\right)$$

$$-\frac{1}{16}\frac{h_x^4}{(j+h_z)^2}\left(\frac{2}{(2j+1-2h_z)^2} + \frac{5}{2j^2} + \frac{2}{(2j-1)^2} - \frac{1}{(j-h_z)^2}\right)$$

$$-\frac{h_x^4}{8}\left(\frac{1}{(j+h_z)^3(2j+1+2h_z)} + \frac{1}{(j+h_z)^2(2j+1+2h_z)^2}\right)$$

$$-\frac{h_x^4}{8}\left(\frac{1}{(j-h_z)^3(2j+1-2h_z)} + \frac{1}{(j-h_z)^2(2j+1-2h_z)^2}\right)$$

$$-\frac{h_x^4}{16}\left(\frac{2}{2j-1} + \frac{1}{j}\right)\left(\frac{1}{(j+h_z)^2(j-h_z)} + \frac{1}{(j+h_z)(j-h_z)^2}\right)$$

$$-\frac{h_x^4}{16}\left(\frac{1}{(j+h_z)(j-h_z)}\left(\frac{4}{(2j-1)^2} + \frac{5}{j^2}\right) + \frac{3h_x^4}{16}\left(\frac{1}{(j+h_z)^4} + \frac{1}{(j-h_z)^4}\right).$$
(92)

The antiphase order parameter for the transverse ANNNI model is given by

$$\rho_{<2>_{tANNNI}} = 1 - \frac{1}{2j^2} h_x^2 - \left(\frac{1 - 16j^2 + 112j^4}{8(4j^2 - 1)^2j^4}\right) h_x^4.$$
(93)

 $\rho_{<2>_{tANNNI}}$ is plotted in figure 3 as a function of h_x for three different values of j. We observe that both the second order and the fourth order contributions to the order parameter are negative, so that the antiphase order parameter drops in value. The vanishing of the order parameter is well depicted in figure 3. The application of an external transverse magnetic field h_x is therefore expected to destroy the <2> antiphase spin ordering which exists at j>0.5 for $h_x = 0$. This expectation turns out to be correct as finite size scaling shows that the model undergoes a transition to paramagnetic phase.



Figure 3: Transverse field antiphase ANNNI order parameter as a function of h_x , to the fourth order, for selected values of j.

4.2.2 Susceptibility

The magnetic susceptiblity of the antiphase ground state under the influence of a weak transverse external magnetic field is

$$\begin{split} \chi_{z_{2>}} &= -2 \frac{\partial^{2} \varepsilon_{z_{2>}}}{\partial \beta^{2}} \bigg|_{\beta=0} \\ &= \frac{1}{2} \bigg(\frac{1}{(j+h_{z})^{3}} + \frac{1}{(j-h_{z})^{3}} \bigg) h_{x}^{2} \\ &+ \bigg\{ \frac{3}{8} \frac{1}{(j+h_{z})^{4}} \bigg(\frac{1}{2j+1+2h_{z}} + \frac{1}{2j} + \frac{1}{2j-1} - \frac{1}{j+h_{z}} \bigg) \\ &+ \frac{3}{8} \frac{1}{(j-h_{z})^{4}} \bigg(\frac{1}{2j+1+2h_{z}} + \frac{1}{2j} + \frac{1}{2j-1} - \frac{1}{j-h_{z}} \bigg) \\ &+ \frac{1}{4} \frac{1}{(j+h_{z})^{2}} \bigg(\frac{2}{(2j+1+2h_{z})^{2}} + \frac{5}{2j^{2}} + \frac{2}{(2j-1)^{2}} - \frac{1}{(j+h_{z})^{2}} \bigg) \\ &+ \frac{1}{4} \frac{1}{(j-h_{z})^{3}} \bigg(\frac{2}{(2j+1-2h_{z})^{2}} + \frac{5}{2j^{2}} + \frac{2}{(2j-1)^{2}} - \frac{1}{(j-h_{z})^{2}} \bigg) \\ &+ \frac{1}{16} \frac{1}{(j-h_{z})^{2}} \bigg(\frac{2}{(2j+1+2h_{z})^{3}} + \frac{13}{j^{3}} + \frac{8}{(2j-1)^{3}} - \frac{2}{(j+h_{z})^{3}} \bigg) \\ &+ \frac{1}{16} \frac{1}{(j+h_{z})^{4}(2j+1+2h_{z})} + \frac{1}{(j-h_{z})^{4}(2j+1-2h_{z})} \bigg) \\ &+ \frac{1}{8} \bigg(\frac{1}{(j+h_{z})^{4}(2j+1+2h_{z})^{2}} + \frac{1}{(j-h_{z})^{4}(2j+1-2h_{z})^{2}} \bigg) \\ &+ \frac{1}{2} \bigg(\frac{1}{(j+h_{z})^{4}(2j+1+2h_{z})^{2}} + \frac{1}{(j-h_{z})^{2}(2j+1-2h_{z})^{2}} \bigg) \\ &+ \frac{1}{2} \bigg(\frac{1}{(j+h_{z})^{4}(2j+1+2h_{z})^{2}} + \frac{1}{(j-h_{z})^{2}(2j+1-2h_{z})^{2}} \bigg) \\ &+ \frac{1}{8} \frac{1}{(j+h_{z})(j-h_{z})} \bigg(\frac{1}{(j+h_{z})^{2}} + \frac{1}{(j-h_{z})^{2}} \bigg) \bigg(\frac{2}{2j-1} + \frac{1}{j} \bigg) \\ &+ \frac{1}{8} \frac{1}{(j+h_{z})(j-h_{z})} \bigg(\frac{1}{(2j-1)^{3}} + \frac{13}{8j^{3}} \bigg) - \frac{3}{4} \bigg(\frac{1}{(j+h_{z})^{5}} + \frac{1}{(j-h_{z})^{5}} \bigg) \bigg\} h_{x}^{4} \,. \tag{94}$$

A particular case of equation (94) is the ANNNI model in a transverse field ($h_z = 0$), for which the magnetic susceptibility is

$$\chi_{<2>_{tANNNI}} = \frac{1}{j^3} h_x^2 + \frac{1}{2j^5} \frac{(-384j^4 + 88j^2 + 832j^6 - 7)}{(4j^2 - 1)^3}.$$
(95)

Again we note that $\chi_{<2>_{tANNNI}}$ is a positive quantity for j > 0.5. The transverse ANNNI model susceptiblity, to fourth order in h_x is plotted in figure 4.



Figure 4: Transverse antiphase ANNNI magnetic susceptibility as a function of h_x , to the fourth order, for selected values of j.

4.2.3 Specific heat

The specific heat of the ANNNI model in the presence of a longitudinal field h_z and a weak transverse field h_x , to second order in h_x is given by

$$c_{<2>} = -\frac{\partial^{2} \varepsilon_{<2>} (\beta = 0)}{\partial h_{x}^{2}}$$

$$= \frac{1}{4} \left(\frac{1}{j+h_{z}} + \frac{1}{j-h_{z}} \right) + \frac{3}{8} \left\{ \frac{1}{(j+h_{z})^{2}} \left(\frac{1}{2j+1+2h_{z}} + \frac{1}{2j} + \frac{1}{2j-1} - \frac{1}{j+h_{z}} \right) \right.$$

$$+ \frac{1}{(j-h_{z})^{2}} \left(\frac{1}{2j+1-2h_{z}} + \frac{1}{2j} + \frac{1}{2j-1} - \frac{1}{j-h_{z}} \right)$$

$$+ \left(\frac{1}{(j+h_{z})^{2} (2j+1+2h_{z})} + \frac{1}{(j-h_{z})^{2} (2j+1-2h_{z})} \right)$$

$$- \left(\frac{1}{(j+h_{z})^{3}} + \frac{1}{(j-h_{z})^{3}} \right) + \frac{1}{(j+h_{z}) (j-h_{z})} \left(\frac{2}{2j-1} + \frac{1}{j} \right) \right\} h_{x}^{2}.$$
(96)

In particular, we have for the ANNNI model in a transverse field, (corresponding to $h_z = 0$ here)

$$c_{<2>_{tANNNI}} = \frac{1}{2j} + \frac{3}{4} \frac{1}{j^3} \left(\frac{4j^2 + 1}{4j^2 - 1} \right) h_x^2 \,. \tag{97}$$

We observe that equation (97) always gives a positive value for the specific heat of the model. We also remark that contrary to the appearance of equation (97), there are no singularities. The condition $2h_z + 1 < 2j$ reduces to j > 0.5 for the unperturbed Hamiltonian (ANNNI model), so that there must be next nearest neighbour interactions and hence j cannot be zero. At j = 0.5, the ground state of the ANNNI model is highly degenerate [10], so that formula (97) is then not valid. The specific heat as a function of h_x is plotted in figure 5 for three different values of j.



Figure 5: Transverse antiphase ANNNI specific heat as a function of h_x , to the fourth order, for selected values of j.

5 The $\uparrow\uparrow\downarrow$ ground state

The ground state of the longitudinal ANNNI model described by the Hamiltonian (1) in the region bounded by the lines $h_z = 1$, $2j+1 = 2h_z$ and $2j+1 = h_z$ is the three-fold degenerate two spins up followed by one spin down state, eigenstates of total S_z with eigenvalue $S_z = N/6$. Classified by translational invariance, these states occur in the k = 0, k = N/3 and k = 2N/3 subspaces of the space of eigenstates of the translation operator T. Here we assume that N is a multiple of 3.

Explicitly, the degenerate states are

$$a\rangle = \frac{1}{\sqrt{3}} \left(\uparrow \uparrow \downarrow \dots \uparrow \uparrow \downarrow \rangle + \left| \uparrow \downarrow \uparrow \dots \uparrow \downarrow \uparrow \rangle + \left| \downarrow \uparrow \uparrow \dots \downarrow \uparrow \uparrow \rangle \right), \tag{98}$$

having translational invariance quantum number k = 0, i.e. the zero momentum state (eigenstate of T of eigenvalue exp(0) = 1).

$$|b\rangle = \frac{1}{\sqrt{3}} \left(|\uparrow\uparrow\downarrow\downarrow\cdots\uparrow\uparrow\downarrow\rangle + \exp(-\frac{2\pi i}{3})|\uparrow\downarrow\uparrow\cdots\uparrow\downarrow\uparrow\rangle + \exp(-\frac{4\pi i}{3})|\downarrow\uparrow\uparrow\cdots\downarrow\uparrow\uparrow\rangle \right), \quad (99)$$

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the $2\pi/3$ -momentum state with k = N/3 (eigenstate of T of eigenvalue $\exp(2\pi i/3)$). and

$$|c\rangle = \frac{1}{\sqrt{3}} \left(\left|\uparrow\uparrow\downarrow\dots\uparrow\uparrow\downarrow\right\rangle + \exp(\frac{2\pi i}{3}) \left|\uparrow\downarrow\uparrow\dots\uparrow\downarrow\uparrow\right\rangle + \exp(\frac{4\pi i}{3}) \left|\downarrow\uparrow\uparrow\dots\downarrow\uparrow\uparrow\right\rangle \right), \quad (100)$$

the $4\pi/3$ -momentum state with k = 2N/3 (eigenstate of T of eigenvalue $\exp(4\pi i/3)$).

The degenerate energy is

$$E_{|a\rangle} = E_{|b\rangle} = E_{|c\rangle} = \frac{-N(1+j+2h_z)}{12}.$$
 (101)

As in the previous section, it is useful to include a symmetry breaking, order parameter term to the Hamiltonian (1) by including a field $\gamma > 0$ and write the unperturbed Hamiltonian as follows:

$$H_{z} = \sum_{i=1}^{N} S_{i}^{z} S_{i+1}^{z} + j \sum_{i=1}^{N} S_{i}^{z} S_{i+2}^{z} - h_{z} \sum_{i=1}^{N} S_{i}^{z} - \gamma \sum_{k=1}^{N/3} \left(S_{3k-2}^{z} + S_{3k-1}^{z} - S_{3k}^{z} \right).$$
(102)

 γ breaks the translational invariance symmetry of H_z , so that the states $|\uparrow\uparrow\downarrow\downarrow\dots\uparrow\uparrow\downarrow\rangle$, $|\uparrow\downarrow\uparrow\dots\uparrow\downarrow\uparrow\rangle$ and $|\downarrow\uparrow\uparrow\dots\downarrow\uparrow\uparrow\rangle$ are no longer degenerate and can therefore no longer be classified as eigenstates of T. The state $|\uparrow\uparrow\downarrow\dots\uparrow\uparrow\downarrow\rangle$ (which we shall henceforth denote by $|\uparrow\uparrow\downarrow\rangle$, with a similar notation for the remaining two states) is now the non-degenerate ground state of H_z .

The long range order parameter $\rho_{\uparrow\uparrow\downarrow}$ and the magnetic susceptibility $\chi_{\uparrow\uparrow\downarrow}$ can now be calculated by computing

$$\rho_{\uparrow\uparrow\downarrow} = -\frac{2}{N} \frac{\partial E_{\uparrow\uparrow\downarrow}(j, h_x, h_z, \gamma)}{\partial \gamma} \bigg|_{\gamma=0}$$
(103)

and

$$\chi_{\uparrow\uparrow\downarrow\downarrow} = -\frac{2}{N} \frac{\partial^2 E_{\uparrow\uparrow\downarrow}(j, h_x, h_z, \gamma)}{\partial \gamma^2} \bigg|_{\gamma=0},$$
(104)

where $E_{\uparrow\uparrow\downarrow}(\gamma=0)$ is the ground state energy of $H = H_z + H_x$ and $\varepsilon_{\uparrow\uparrow\downarrow}(\gamma=0)$ the ground state energy per spin. To zeroth order then,

$$E_{\uparrow\uparrow\downarrow}^{(0)}(j,h_x = 0,h_z,\gamma) = \frac{-N(1+j+2h_z)}{12} - \frac{N\gamma}{2}$$
(105)

and

$$E_{\uparrow\downarrow\uparrow}^{(0)}(j,0,h_{z},\gamma) = \frac{-N(1+j+2h_{z})}{12} + \frac{N\gamma}{6} = E_{\downarrow\uparrow\uparrow}^{(0)}(j,0,h_{z},\gamma).$$
(106)

5.1 Energy corrections

5.1.1 First order correction to the ground state energy

Since the three states $|\uparrow\uparrow\downarrow\rangle$, $|\uparrow\downarrow\uparrow\rangle$ and $|\downarrow\uparrow\uparrow\rangle$ are degenerate for $\gamma = 0$, we can consider γ to be small and attempt to apply degenerate perturbation theory to determine the first order corrections to the energies. The 3×3 perturbation matrix $V^{(1)}$ is given by

$$V^{(1)} = \begin{pmatrix} \langle \uparrow \uparrow \downarrow | H_x | \uparrow \uparrow \downarrow \rangle & \langle \uparrow \uparrow \downarrow | H_x | \uparrow \downarrow \uparrow \rangle & \langle \uparrow \uparrow \downarrow | H_x | \downarrow \uparrow \uparrow \rangle \\ \langle \uparrow \downarrow \uparrow | H_x | \uparrow \uparrow \downarrow \rangle & \langle \uparrow \downarrow \uparrow | H_x | \uparrow \downarrow \uparrow \rangle & \langle \uparrow \downarrow \uparrow | H_x | \downarrow \downarrow \uparrow \rangle \\ \langle \downarrow \uparrow \uparrow | H_x | \uparrow \uparrow \downarrow \rangle & \langle \downarrow \uparrow \uparrow | H_x | \uparrow \downarrow \uparrow \rangle & \langle \downarrow \uparrow \uparrow | H_x | \downarrow \uparrow \uparrow \rangle \\ \langle \downarrow \uparrow \uparrow | H_x | \uparrow \uparrow \downarrow \rangle & \langle \downarrow \uparrow \uparrow | H_x | \uparrow \downarrow \uparrow \rangle & \langle \downarrow \uparrow \uparrow | H_x | \downarrow \uparrow \uparrow \rangle \end{cases}$$

But the three states $|\uparrow\uparrow\downarrow\rangle$, $|\uparrow\downarrow\uparrow\rangle$ and $|\downarrow\uparrow\uparrow\rangle$ are all eigenstates of total S_z with the same eigenvalue of $S_z = N/6$ for a chain of N spins, it follows from equation (12) that $V^{(1)}$ is a null matrix, so that there are no first order contributions to the energies.

(107)

5.1.2 Second order correction to the ground state energy

Treating γ as a small parameter and the states $\{\uparrow\uparrow\downarrow\downarrow\rangle, |\uparrow\downarrow\uparrow\downarrow\rangle, |\downarrow\uparrow\uparrow\rangle\}$ as nearly degenerate, the 3×3 second order perturbation matrix $V^{(2)}$ has elements of the form

$$V_{ij}^{(2)} = \sum_{k} \frac{\langle i | H_x | k \rangle \langle k | H_x | j \rangle}{E_i^{(0)} - E_k^{(0)}},$$
(108)

where

$$i, j \in \{\uparrow\uparrow\downarrow\rangle, |\uparrow\downarrow\uparrow\rangle, |\downarrow\uparrow\uparrow\rangle\},$$

and k runs over the 2^{N} basis states of the Hilbert space excluding $|i\rangle$ and $|j\rangle$. Clearly, for $i \neq j$, any state $|k\rangle$ whose H_{x} matrix element with $|i\rangle$ must have a vanishing matrix element with $|j\rangle$. Therefore the matrix $V^{(2)}$ is diagonal, with the diagonal elements giving the second order corrections to the ground state energies. That is

$$V_{11}^{(2)} = E_{\uparrow\uparrow\downarrow}^{(2)} = \sum_{k} \frac{\left| \left\langle \uparrow\uparrow\downarrow \left| H_{x} \right| k \right\rangle \right|^{2}}{E_{\uparrow\uparrow\downarrow}^{(0)} - E_{k}^{(0)}},$$
(109)

$$V_{22}^{(2)} = E_{\uparrow\downarrow\uparrow}^{(2)} = \sum_{k} \frac{\left|\left\langle\uparrow\downarrow\uparrow\left|H_{x}\right|k\right\rangle\right|^{2}}{E_{\uparrow\downarrow\uparrow}^{(0)} - E_{k}^{(0)}}$$
(110)

and

$$V_{33}^{(2)} = E_{\downarrow\uparrow\uparrow}^{(2)} = \sum_{k} \frac{\left| \left\langle \downarrow\uparrow\uparrow \left| H_{x} \right| k \right\rangle \right|^{2}}{E_{\downarrow\uparrow\uparrow}^{(0)} - E_{k}^{(0)}} \,. \tag{111}$$

We note that there are only N non-vanishing contributions in each of the above sums, so that the evaluation of each sum is almost trivial. We have

$$E_{\uparrow\uparrow\downarrow}^{(2)}(j,h_x,h_z,\gamma) = -\frac{Nh_x^2}{12} \left(\frac{2}{h_z + \gamma} + \frac{1}{1 + j - h_z + \gamma}\right)$$
(112)

and

$$E_{\uparrow\downarrow\uparrow}^{(2)}(j,h_x,h_z,\gamma) = -\frac{Nh_x^2}{12} \left(\frac{1}{h_z+\gamma} + \frac{1}{1+j-h_z-\gamma} + \frac{1}{h_z-\gamma}\right) = E_{\downarrow\uparrow\uparrow\uparrow}^{(2)}(\gamma).$$
(113)

We see here that the degeneracy in the states $|\uparrow\downarrow\uparrow\rangle$ and $|\downarrow\uparrow\uparrow\rangle$ is not lifted to second order in h_x .

5.1.3 Fourth order correction

The fourth order correction to the energy of the $|\uparrow\uparrow\downarrow\rangle$ state is given by

$$E_{\uparrow\uparrow\downarrow\downarrow}^{(4)} = \sum_{ijk} \frac{\left\langle \uparrow\uparrow\downarrow \left|H_{x}\right| i\right\rangle \langle i\left|H_{x}\right| j\right\rangle \langle j\left|H_{x}\right| k\right\rangle \langle k\left|H_{x}\right| \uparrow\uparrow\downarrow\rangle}{(E_{\uparrow\uparrow\downarrow\downarrow}^{(0)} - E_{i}^{(0)})(E_{\uparrow\uparrow\downarrow\downarrow}^{(0)} - E_{j}^{(0)})(E_{\uparrow\uparrow\downarrow\downarrow}^{(0)} - E_{k}^{(0)})} - E_{i\uparrow\downarrow\downarrow}^{(0)} \sum_{k} \frac{\left\langle \uparrow\uparrow\downarrow \left|H_{x}\right| k\right\rangle \langle k\left|H_{x}\right| \uparrow\uparrow\downarrow\rangle}{(E_{\uparrow\uparrow\downarrow\downarrow}^{(0)} - E_{k}^{(0)})^{2}}.$$
(114)

If we let $\{|a_r\rangle, r = 1, 2, \dots, N\}$ be the set of states such that $\langle \uparrow \uparrow \downarrow | H_x | a_r \rangle \neq 0$,

that is if

$$|a_{r}\rangle \in \{ |\uparrow\uparrow\downarrow\downarrow\dots\uparrow\uparrow\downarrow\uparrow\uparrow\uparrow\rangle, |\uparrow\uparrow\downarrow\downarrow\dots\uparrow\uparrow\downarrow\downarrow\downarrow\rangle, |\uparrow\uparrow\downarrow\downarrow\dots\uparrow\uparrow\downarrow\downarrow\uparrow\downarrow\rangle, |\uparrow\uparrow\downarrow\downarrow\downarrow\uparrow\downarrow\rangle, |\uparrow\uparrow\downarrow\downarrow\downarrow\uparrow\downarrow\rangle, |\uparrow\uparrow\downarrow\downarrow\uparrow\downarrow\rangle, |\uparrow\uparrow\downarrow\downarrow\uparrow\downarrow\rangle\rangle, |\uparrow\uparrow\uparrow\downarrow\downarrow\downarrow\uparrow\uparrow\downarrow\rangle\rangle, |\uparrow\uparrow\uparrow\downarrow\downarrow\uparrow\uparrow\downarrow\rangle\rangle, |\uparrow\uparrow\uparrow\downarrow\uparrow\downarrow\rangle\rangle, |\uparrow\uparrow\uparrow\downarrow\uparrow\uparrow\downarrow\rangle\rangle, |\uparrow\uparrow\uparrow\uparrow\downarrow\rangle\rangle\rangle \},$$
(116)

then equation (114) simplifies to

$$E_{\uparrow\uparrow\downarrow\downarrow}^{(4)} = \sum_{rs} \left(\frac{\left\langle \uparrow\uparrow\downarrow \middle| H_x \middle| a_r \right\rangle \left\langle a_r \middle| H_x \middle| \uparrow\uparrow\downarrow \right\rangle}{(E_{\uparrow\uparrow\downarrow}^{(0)} - E_{a_r}^{(0)})(E_{\uparrow\uparrow\downarrow}^{(0)} - E_{a_s}^{(0)})} \sum_j \frac{\left\langle a_r \middle| H_x \middle| j \right\rangle \left\langle j \middle| H_x \middle| a_s \right\rangle}{E_{\uparrow\uparrow\downarrow\downarrow}^{(0)} - E_j^{(0)}} \right) - E_{\uparrow\uparrow\downarrow\downarrow}^{(0)} \sum_r \frac{\left| \left\langle \uparrow\uparrow\downarrow \middle| H_x \middle| a_r \right\rangle \right|^2}{(E_{\uparrow\uparrow\downarrow\downarrow}^{(0)} - E_{a_r}^{(0)})^2} .$$

$$(117)$$

Maple procedures evaluate the above sums as s_1 and s_2 , respectively, where

$$\frac{16s_{1}}{h_{x}^{4}} = \frac{2N}{3} \frac{1}{(-h_{z} - \gamma)^{2}} \left\{ \frac{1}{-1 - 2h_{z} - 2\gamma} + \frac{1}{-1 - 2\gamma} + \frac{1}{-j - 2\gamma} + \frac{2N/3 - 3}{-2h_{z} - 2\gamma} + \frac{N/3 - 2}{-2h_{z} - 2\gamma} + \frac{1}{-j - 2h_{z} - 2\gamma} \right\} + \frac{N/3(N/3 - 1)}{(-1 - j + h_{z} - \gamma)^{2}(-2 - 2j + 2h_{z} - 2\gamma)} + \frac{N}{3} \frac{1}{(-1 - j + h_{z} - \gamma)^{2}} \left\{ \frac{2}{-1 - 2\gamma} + \frac{2}{-j - 2\gamma} + \frac{2N/3 - 4}{-1 - j - 2\gamma} + \frac{N/3 - 1}{-2 - 2j + 2h_{z} - 2\gamma} \right\} + \frac{1}{(-h_{z} - \gamma)^{2}} \left\{ \frac{2N/3}{-1 - 2h_{z} - 2\gamma} + \frac{2N/3(2N/3 - 3)}{-2h_{z} - 2\gamma} + \frac{2N/3}{-j - 2h_{z} - 2\gamma} \right\} + \frac{1}{(-h_{z} - \gamma)(-1 - j + h_{z} - \gamma)} \left\{ \frac{4N/3}{-1 - 2\gamma} + \frac{4N/3(N/3 - 2)}{-1 - j - 2\gamma} + \frac{4N/3}{-j - 2\gamma} \right\}$$
(118)

and

(115)

$$\frac{16s_2}{h_x^4} = -\left(\frac{2N}{3}\frac{1}{\left(-h_z - \gamma\right)^2} + \frac{N}{3}\frac{1}{\left(-1 - j + h_z - \gamma\right)^2}\right)\left(\frac{2N}{3}\frac{1}{-h_z - \gamma} + \frac{N}{3}\frac{1}{-1 - j + h_z - \gamma}\right).$$
 (119)

Upon adding equations (118) and (119) and noting the cancellation of the terms proportional to N^2 , we obtain

$$\mathcal{E}_{\uparrow\uparrow\downarrow\downarrow}^{(4)}(j,h_x,h_z,\gamma) = \frac{h_x^4}{12} \frac{1}{(h_z+\gamma)^2} \left\{ -\frac{1}{(1+2h_z+2\gamma)} + \frac{3}{2h_z+2\gamma} - \frac{1}{j+2h_z+2\gamma} \right\}$$

+ $\frac{h_x^4}{24} \left\{ \frac{1}{(h_z+\gamma)^2} + \frac{1}{(1+j-h_z+\gamma)^2} + \frac{2}{(h_z+\gamma)(1+j-h_z+\gamma)} \right\} \times$
 $\left\{ -\frac{1}{1+2\gamma} - \frac{1}{j+2\gamma} + \frac{2}{1+j+2\gamma} \right\} + \frac{h_x^4}{48} \frac{1}{(1+j-h_z+\gamma)^3},$ (120)

so that the fourth order correction to the ground state energy per spin of the $\uparrow\uparrow\downarrow$ state is given by

$$\mathcal{E}_{\uparrow\uparrow\downarrow}^{(4)}(j,h_x,h_z,0) = \frac{h_x^4}{12} \frac{1}{h_z^2} \left\{ -\frac{1}{1+2h_z} + \frac{3}{2h_z} - \frac{1}{j+2h_z} \right\}$$

$$+ \frac{h_x^4}{24} \left\{ \frac{1}{h_z^2} + \frac{1}{(1+j-h_z)^2} + \frac{2}{h_z(1+j-h_z)} \right\} \left\{ -1 - \frac{1}{j} + \frac{2}{1+j} \right\}$$

$$+ \frac{h_x^4}{48} \frac{1}{(1+j-h_z)^3}.$$

$$(121)$$

Combining equations (105), (112) and (120), we have

$$\mathcal{E}_{\uparrow\uparrow\downarrow}(j,h_x,h_z,\gamma) = \frac{h_x^4}{12} \frac{1}{(h_z+\gamma)^2} \left\{ -\frac{1}{(1+2h_z+2\gamma)} + \frac{3}{2h_z+2\gamma} - \frac{1}{j+2h_z+2\gamma} \right\}$$

$$+ \frac{h_x^4}{24} \left\{ \frac{1}{(h_z+\gamma)^2} + \frac{1}{(1+j-h_z+\gamma)^2} + \frac{2}{(h_z+\gamma)(1+j-h_z+\gamma)} \right\} \times$$

$$\left\{ -\frac{1}{1+2\gamma} - \frac{1}{j+2\gamma} + \frac{2}{1+j+2\gamma} \right\} + \frac{h_x^4}{48} \frac{1}{(1+j-h_z+\gamma)^3}$$

$$- \frac{h_x^2}{12} \left\{ \frac{2}{h_z+\gamma} + \frac{1}{1+j-h_z+\gamma} \right\} - \frac{(1+j+2h_z)}{12} - \frac{\gamma}{2}.$$

$$(122)$$

The ground state energy of the longitudinal ANNNI model in the region bounded by the lines $2j + h_z = 1$, $h_z = 1$ and $2h_z + 1 = 2j$, to fourth order in h_x is therefore given by

$$\mathcal{E}_{\uparrow\uparrow\downarrow}(j,h_x,h_z,0) = \frac{h_x^4}{12} \frac{1}{h_z^2} \left\{ -\frac{1}{1+2h_z} + \frac{3}{2h_z} - \frac{1}{j+2h_z} \right\} + \frac{h_x^4}{24} \left\{ \frac{1}{h_z^2} + \frac{1}{(1+j-h_z)^2} + \frac{2}{h_z(1+j-h_z)} \right\} \left\{ -1 - \frac{1}{j} + \frac{2}{1+j} \right\} + \frac{h_x^4}{48} \frac{1}{(1+j-h_z)^3} - \frac{h_x^2}{12} \left(\frac{2}{h_z} + \frac{1}{1+j-h_z} \right) - \frac{(1+j+2h_z)}{12}.$$
(123)

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As noted earlier, the $\uparrow\uparrow\downarrow$ state as an eigenstate of the unperturbed Hamiltonian h_z has the unique property that it can be ground state only for finite h_z and finite j (in fact j > 0.5). If j = 0, the ground state is ferromagnetic for $h_z > 1$ and antiferromagnetic otherwise. If $h_z = 0$ the ground state is the four-fold degenerate antiphase configuration for j > 0.5 and the two-fold degenerate configuration if j < 0.5. One implication of this remark is that there are no special cases of equation (123).

Typical behaviour of $\varepsilon_{\uparrow\uparrow\downarrow}(j,h_x,h_z,0)$ as a function of h_x is plotted in figures 6a and 6b. Comparing the two curves, it appears that $\varepsilon_{\uparrow\uparrow\downarrow}(j,h_x,h_z,0)$ is more sensitive to changes in *j* than in h_z .



(b) $\mathcal{E}_{\uparrow\uparrow\downarrow}(j, h_x, h_z, 0)$ as a function of h_x for j = 0.5

Figure 6: $\varepsilon_{\uparrow\uparrow\downarrow}(j,h_x,h_z,0)$ as a function of h_x

5.2 Physical quantities

5.2.1 Long range order parameter

From equations (103), (104) and (122) we obtain the long range order parameter $\rho_{\uparrow\uparrow\downarrow}$ of the $\uparrow\uparrow\downarrow$ state to fourth order in the perturbation h_x as

$$\rho_{\uparrow\uparrow\downarrow} = 1 - \frac{h_x^2}{6} \left(\frac{2}{h_z^2} + \frac{1}{(1+j-h_z)^2} \right) + \frac{h_x^4}{3h_z^3} \left(-\frac{1}{1+2h_z} + \frac{3}{2h_z} - \frac{1}{j+2h_z} \right) - \frac{h_x^4}{6h_z^2} \left(\frac{2}{(1+2h_z)^2} - \frac{3}{2h_z^2} + \frac{2}{(j+2h_z)^2} \right) + \frac{1}{8} \frac{h_x^4}{(1+j-h_z)^4} - 2h_x^4 \left(\frac{1}{h_z^3} + \frac{1}{(1+j-h_z)^3} + \frac{1}{h_z^2(1+j-h_z)} + \frac{1}{h_z(1+j-h_z)^2} \right) \left(-1 - \frac{1}{j} + \frac{2}{1+j} \right) - \frac{h_x^4}{6} \left(\frac{1}{h_z^2} + \frac{1}{(1+j-h)^2} + \frac{2}{h_z(1+j-h_z)} \right) \left(1 + \frac{1}{j^2} - \frac{2}{(1+j)^2} \right)$$
(124)

A typical behaviour of the long range order parameter is depicted in figure 7. To fourth order in perturbation, we see that the $\uparrow\uparrow\downarrow$ order of the ANNNI model in mixed fields vanish. That the model indeed does not possess long range order in the thermodynamic limit was confirmed by finite size scaling results which showed that the model indeed undergoes a phase transition from the $\uparrow\uparrow\downarrow$ state to a paramagnetic phase.



Figure 7: $\rho_{\uparrow\uparrow\downarrow}$ as a function of h_x to fourth order in h_x

CONCLUSION

Using Rayleigh-Schrödinger perturbation theory, we have derived analytic expressions for the ground state energy of the ANNNI model in two perpendicular fields, as a function of the nearest neighbour exchange interaction j and the two fields h_x and h_y . The transverse field h_x was taken as the perturbation parameter, and the calculation was done to the fourth order in hx. The motivation was the fact that many important physical quantities, such as magnetization, of a statistical system, can be determined once the ground state energy is known.

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