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Order and Disorder Lines in Systems with Competing Interactions: I. Quantum Spins at $T = 0$

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In the parameter space of systems with competing interactions there are specific trajectories called order (disorder) lines. Along these trajectories the competition between the different interactions effectively reduces the dimensionality of the system and the model can be exactly solved. It is shown that the order (disorder) trajectories end up at a multicritical point. The method of Peschel and Emery is used to determine the (anisotropic) critical behavior of the spin–spin correlation functions near the multicritical point. The quantum spin systems discussed here include the XYZ chain in a field, the straggered XYZ chain in a field, and a Hamiltonian version of a three-dimensional Ising model with biaxial competing interactions.

KEY WORDS: Quantum spin systems; order; disorder; kinetic Ising model; duality transformation; Hamiltonian limit.

1. INTRODUCTION

In a remarkable paper Peschel and Emery (PE)[1] have recently shown how to determine disorder lines in quantum spin chains. Their method is based on the fact that for a special choice of the coupling constants the Hamiltonian can be interpreted as the time evolution (Liouville) operator of the kinetic Ising model. This mapping holds on a given trajectory of the parameter space, called a disorder line (DOL) if the ground state is not degenerate (disordered phase) and an order line (OL) if the ground state is degenerate (usually a ferromagnetic phase).

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There are disparate results in the literature regarding disorder (order) lines. They had been obtained maninly for the free-fermion models (anisotropic antiferromagnetic triangular Ising model,[2] the kagomé Ising model,[3] the quantum XY chain[4]). These results will be used to conjecture the properties of spin–spin correlation functions when the temperaturelike parameter is changed near a disorder (order) line.

The main conclusion of this series of papers is that the presence of DOL (OL) is a common phenomenon in models with competing interactions. The determination of these trajectories is very helpful for the construction of the phase diagrams and in the interpretation of experiments or Monte Carlo simulations. Moreover, the spin–spin correlation length may have a nonanalytic behavior along the DOL (OL), affecting the validity of high- (low-) temperature expansions. A detailed discussion of the general properties of DOL (OL) is given in Section 5.

In this paper we discuss quantum $1/2$-spin models at $T = 0$. The significance of these models is twofold. First, one has many real life magnetic materials which have a quasi-one-dimensional behavior.[5,6] Also, the spin-$1/2$ chain Hamiltonian is relevant for a variety of other systems, including highly conductive organic materials[7] or different quasi-one-dimensional systems bearing charge and/or spin density waves. On the other hand, d-dimensional quantum spin Hamiltonians at $T = 0$ can be related through the transfer matrix formalism to $(d + 1)$-dimensional Ising-like models. For instance, the XYZ-chain Hamiltonian commutes with the transfer matrix of the eight-vertex model.[8,9] A less rigorous but more general relationship between transfer matrices of $(d + 1)$-dimensional Ising-like systems and d-dimensional quantum Hamiltonians at $T = 0$ is obtained in the so-called Hamiltonian limit.[10] In this paper the PE method is used to determine DOL (OL) in the Hamiltonian limit of two- and three-dimensional Ising models with competing interactions, while in the succeeding paper a different method is used directly within the tranfer matrix formalism and is applied to the IRF (interactions-around-a-face) model, including the eight-vertex model.[11]

Our results are presented in the following order. In Section 2 the PE method is reviewed and applied to the XYZ chain in a field. The free-fermion case is discussed in detail as well as how the duality transformation maps the DOL into the OL. In Section 3, it is shown that the disorder trajectories end on a line of multicritical points. The critical exponents of the correlation length along the chain is $\nu_{\|} = 1$, while in the direction perpendicular to the chain ("time direction") one finds $\nu_{\perp} = z \cdot \nu_{\|}$, where z is the usual dynamic exponent.[12] The order trajectories also end on multicritical points, but with different critical properties.

In Section 4 the PE method is applied to a staggered (dimerized) XYZ chain in a field and to the Hamiltonian limit of a three-dimensional Ising model on a hexagonal lattice with biaxial competing interactions. For this model one obtains a multicritical point with a characteristic anisotropic character ($\nu_{\parallel} = 1$, $\nu_{\perp} = 2.125$) at a finite temperature. A generalization of the concept of DOL (OL) and a discussion of their general properties is given in Section 5.

2. THE PESCHEL–EMERY METHOD AND THE XYZ CHAIN IN A FIELD

Consider first the one-dimensional Ising model:

$$-\beta H^{\text{eff}} = K \sum_j s_j s_{j+1} \tag{2.1}$$

where $\beta = 1/k_B T$ and $s_j = \pm 1$. Following Glauber,[13] a master equation for the time-dependent distribution function $\Psi(\{s_j\}, t)$ can be written for the discrete Markoff process involving single spin flips[14]:

$$\frac{d}{dt}\Psi = -L\Psi \tag{2.2}$$

where

$$L = \sum_j w_j^{1/2}(1 - \hat{P}_j) w_j^{1/2} \tag{2.3}$$

Here $w_j = w_j(s_{j-1}, s_j, s_{j+1})$ gives the transition probability that s_j changes into $-s_j$ in a given time period. $\hat{P}_j$ is the spin flip operator $\hat{P}_j s_j = -s_j$. A general choice of w_j satisfying the detailed balance condition is

$$w_j = f_j \exp(-s_j h_j) \geqslant 0 \tag{2.4}$$

where $h_j = h_j(s_{j-1}, s_{j+1})$ is the factor of s_j in (2.1) and f_j is a non-negative function of the spins nearest neighbors to s_j:

$$f_j = \left(\frac{\alpha_0 + \alpha_1}{2} + \frac{\alpha_0 - \alpha_1}{2} s_{j-1} s_{j+1} \right), \qquad \alpha_0, \alpha_1 \geqslant 0 \tag{2.5}$$

From (2.3) and (2.4) one gets

$$L = \sum_j f_j [\exp(-s_j h_j) - P_j] \tag{2.6}$$

One makes the connection to the quantum formalism[15] by writing

$$\Psi(s_1, s_2, \ldots, s_N) = \Psi(\sigma_1^z, \sigma_2^z, \ldots, \sigma_N^z)|0_+\rangle \tag{2.7}$$

$$|0_+\rangle = \sum_{s_j = \pm 1} |s_1\rangle |s_2\rangle \cdots |s_N\rangle = \prod_j \otimes \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}_j \tag{2.8}$$

and

$$P_j = \sigma_j^x \tag{2.9}$$

Here σ^x and σ^z are the usual Pauli matrices. Note that $\sigma_j^x|0_+\rangle = |0_+\rangle$ for all $j = 1, 2, \ldots, N$. The Liouville operator L (2.6) is rewritten as

$$L = \sum_j (A\sigma_{j-1}^z\sigma_{j+1}^z + B\sigma_j^z\sigma_{j+1}^z + C\sigma_j^x + D\sigma_{j-1}^z\sigma_j^x\sigma_{j+1}^z) \tag{2.10}$$

where

$$\begin{aligned} A &= \tfrac{1}{2}(\alpha_1 - \alpha_0 \cosh 2K) \\ B &= -\alpha_0 \sinh 2K \\ C &= -\tfrac{1}{2}(\alpha_0 + \alpha_1) \\ D &= -\tfrac{1}{2}(\alpha_0 - \alpha_1) \end{aligned} \tag{2.11}$$

Implementing the duality transformation[16] by introducing the bond Pauli operators,

$$\tau_{j+1/2}^z = \sigma_j^z\sigma_{j+1}^z \tag{2.12a}$$

$$\tau_{j+1/2}^x = \prod_{k \leqslant j} \sigma_k^x \tag{2.12b}$$

one obtains the dual operator of L:

$$L^D = \sum_j (A\tau_j^z\tau_{j+1}^z + B\tau_j^z + C\tau_j^x\tau_{j+1}^x - D\tau_j^y\tau_{j+1}^y) \tag{2.13}$$

Consider next the XYZ chain Hamiltonian in the following parameterization:

$$H_{XYZ} = -\sum_j \{J[(1+\gamma)\tau_j^x\tau_{j+1}^x + (1-\gamma)\tau_j^y\tau_{j+1}^y + \Delta\tau_j^z\tau_{j+1}^z] + 2h\tau_j^z\} \tag{2.14}$$

where without loss of generality we take $\gamma \geqslant 0$. This Hamiltonian commutes with the transfer matrix of the symmetric eight-vertex model[8,9] if $h = 0$. The ground state energy and the elementary excitations can be calculated using Baxter's solution.[17,18] When $\gamma = 0$ the H_{XXZ} Hamiltonian commutes with the transfer matrix of a six-vertex model.[11,19] The ground state and the low-lying excitations can be calculated using the Bethe-ansatz method.[20,21] Finally, if $\Delta = 0$ (2.14) describes an XY chain which has been considered by different authors.[22,23] In particular, the spin–spin correlation functions have been calculated by Niemeijer[24] and by Barouch and McCoy.[4] For $\Delta = 0$, $h^2 + \gamma^2 \geqslant 1$ Suzuki[25] proved that (2.14) commutes with the transfer matrix of an anisotropic square Ising model.

Applying the inverse of the duality transformation (2.12) to (2.14) one obtains the dual of the H_{XYZ} as

$$H^D_{XYZ} = -\sum_j \{J[(1+\gamma)\sigma^x_j + (\gamma-1)\sigma^z_{j-1}\sigma^x_j\sigma^z_{j+1} + \Delta\sigma^z_{j-1}\sigma^z_{j+1}] + 2h\sigma^z_j\sigma^z_{j+1}\} \tag{2.15}$$

For $\Delta = 0$ Stephen and Mittag have shown that H^D_{XY} commutes with the diagonal-to-diagonal transfer matrix of the triangular Ising model.[26] The correlation functions of (2.15) for $\Delta = 0$ are related to the correlation functions of the triangular Ising model calculated by Stevenson.[2]

By comparing (2.10) (or (2.13)) to (2.15) (or (2.14)) it is clear that if

$$\begin{aligned} 1+\gamma &= \tfrac{1}{2}(\alpha_0+\alpha_1) \\ 1-\gamma &= \tfrac{1}{2}(\alpha_1-\alpha_0) \\ \Delta &= \tfrac{1}{2}(\alpha_1 - \alpha_0\cosh 2K) \\ 2h/J &= \alpha_0 \sinh 2K \end{aligned} \tag{2.16}$$

the operator H^D_{XYZ} (H_{XYZ}) is identical to L (L^D) except for a constant factor and a constant shift of the ground state energy. By eliminating α_0, α_1, and K from (2.16) this happens on the surface:

$$\begin{aligned} &\gamma^2 + (h/J)^2 = (\Delta-1)^2 \\ &\Delta \leqslant 1-\gamma \qquad (K \text{ is real}) \end{aligned} \tag{2.17}$$

It follows that the ground state of L

$$\Psi_{\text{eq}} = \exp\left(\frac{K}{2}\sum_j s_j s_{j+1}\right) = |\Psi_0\rangle = \exp\left(\frac{K}{2}\sum \sigma^z_j\sigma^z_{j+1}\right)|0_+\rangle \tag{2.18}$$

is also the ground state of H^D_{XYZ} on the surface (2.17), which is shown in Fig. 1. The ground state (2.18) is unique and therefore (2.17) represents a *disorder* line in H^D_{XYZ}.

Assuming periodic boundary conditions the transformation (2.12a) maps $\sum\sigma^z_j\sigma^z_{j+1}$ into $\sum\tau^z_j$, while the transformation (2.12b) maps the state $|0_+\rangle$ into itself or into the state $|0_-\rangle$, where $\tau^x_j|0_-\rangle = -|0_-\rangle$ for all $j = 1, 2, \ldots, N$. Taking into accunt also the parity of the ground state (2.18), one finds that the ground state of L^D (H_{XYZ}) is given by

$$|\Psi^D_0\rangle = \exp\left(\frac{K}{2}\sum\tau^z_j\right)(|0_+\rangle + |0_-\rangle) \tag{2.19}$$

and is degenerate with the state

$$|\Psi^D_0\rangle_- = \exp\left(\frac{K}{2}\sum\tau^z_j\right)(|0_+\rangle - |0_-\rangle) \tag{2.20}$$

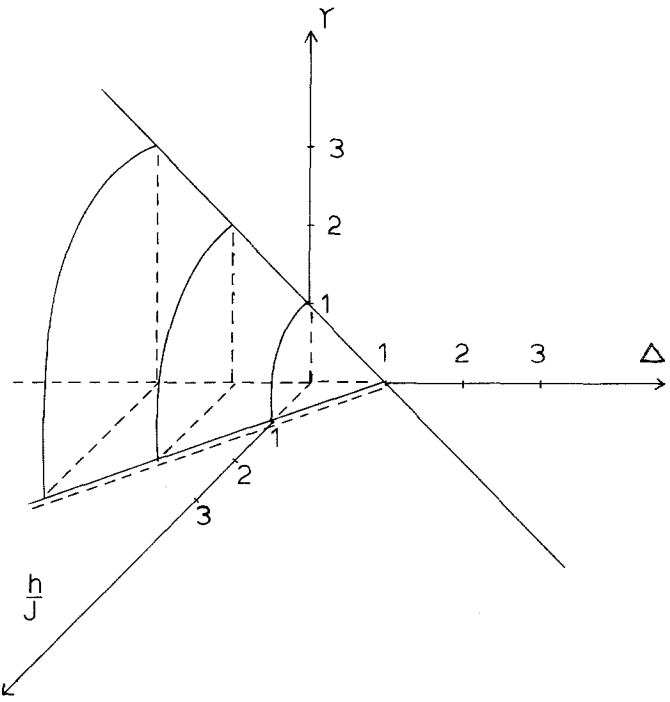

Fig. 1. The order (disorder) surface in the H_{XYZ} (H^D_{XYZ}). Except for the line $h/J = 0$, $\Delta = 1 - \gamma$, it is a cone ending on the Heisenberg point $\Delta = 1$, $h/J = 0$, $\gamma = 0$. The line of multicritical points $\gamma = 0$ is shown by a dotted line.

Accordingly, the trajectory (2.17) is called an *order* line in H_{XYZ} or L^D. Note that $\langle \Psi_0 | \Psi_0 \rangle$ is just the partition function of a one-dimensional Ising chain (2.1) with nearest-neighbor (n.n.) interactions, while $\langle \Psi_0^D | \Psi_0^D \rangle$ is the partition function of noninteracting Ising spins in an external field.

The order (disorder) surface is the half-cone shown in Fig. 1. At $\Delta = 0$ the *order* line was found by Barouch and McCoy.[4] Its dual counterpart, the *disorder* line for $\Delta = 0$, was discussed by Stevenson[2] and has exactly the form (2.17).[1] These calculations revealed also a very interesting property of the correlation functions. The correlation functions have the usual exponential decay *outside* the cone but are modulated by a varying characteristic wave vector inside the cone. This feature is probably present also for $\Delta \neq 0$. Another interesting result of the free fermion calculations[2] on H^D_{XYZ} is that the correlation length between spins along the chain, $\xi_{\|}$, has a cusplike minimum. This involves a nonanalytic behavior on (2.17), which had been also found in the XY model.[4] In Section 5 we shall

present some general arguments favoring the view that exact high- (low-) temperature expansions are not convergent on the disorder (order) surfaces.

3. CRITICAL BEHAVIOR NEAR MULTICRITICAL POINTS

Consider first the operator H^D_{XYZ} (2.15). Its ground state behaves effectively as the one-dimensional Ising model (2.1) on the disorder surface (2.17). This underlying model, in turn, exhibits a phase transition at $K = \pm\infty$. From (2.16) this happens for

$$\gamma = 0, \qquad h = \pm J(1 - \Delta) \tag{3.1}$$

or

$$0 < \gamma < \infty, \quad \Delta \to -\infty, \quad \frac{h}{J} \to \pm\infty, \quad \text{but} \quad \frac{h}{J} = \pm|\Delta| \tag{3.2}$$

The lines (3.1) and (3.2) are lines of multicritical points and all these points have critical properties similar to the $T = 0$ multicritical point of the axial next-nearest-neighbor Ising (ANNNI) model.[1,27,28]

The spin–spin correlation function along the chain is given by

$$G^{\|}_R(z) = \frac{\langle \Psi_0 | \sigma^z_0 \sigma^z_R | \Psi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle} \tag{3.3}$$

On the disorder surface (2.17) it corresponds to the spin–spin correlation function of the one-dimensional Ising model (2.1). Using Eqs. (2.16) one finds s that

$$\xi_{\|} \sim \gamma^{-\nu_{\|}} = \gamma^{-1} \tag{3.4}$$

when $\gamma \to 0_+$ along (2.17). A similar result ($\nu_{\|} = 1$) holds when approaching the multicritical line (3.2).

A remarkable advantage of the Peschel–Emery method is that it allows also for the calculation of the correlation length in the direction perpendicular to the chain (y or "time" direction). From the Hamiltonian limit formalism[10] it follows that one might interpret the H^D_{XYZ} Hamiltonian as the extreme anisotropic limit of a two-dimensional Ising spin model with multiple interactions (see also the following paper). The correlation length in the direction perpendicular to the chain is then related to the inverse of the mass gap:

$$\xi_{\perp}^{-1} \simeq E_1 - E_0 \sim \tau^{-1} \tag{3.5}$$

Since on (2.17) the spectra of H^D_{XYZ} and L are identical, so is the mass gap (3.5). On the other hand, the mass gap of the Liouville operator (2.6) corresponds to the inverse of the longest relaxation time, τ, which diverges at $|K| \to \infty$ with the dynamic exponent $\Delta = z\nu_{\|}$. Therefore the correlation

function between spins in the direction perpendicular to the competition axis shows a singular behavior related to the dynamic slowing down of the effective Ising model (2.1). In our case $z = 3$, $\nu_{\parallel} = 1$, so

$$\xi_{\perp} \sim \gamma^{-\nu_{\perp}} \sim \gamma^{-3} \tag{3.6}$$

for $\gamma \to 0_+$ on (2.17). The peculiar value $z = 3$[29] (the "normal" value in one dimension is $z = 2$ for the Glauber model) is due to the fact that as $\gamma \to 0_+$ the factor f_j (2.5) becomes zero for every configuration of clusters with at least two parallel nearest-neighbor spins. All these states are then frozen in the ground state of L, which corredponds—not accidentally—to the $T = 0$ multicritical point of the ANNNI model.[1,30]

What is the corresponding behavior for *order* lines, that is, for the operator H_{XYZ} on (2.17)? In this case the ground state represents the Boltzmann distribution of an Ising model in an external field. Therefore the spin–spin correlation function $G_R^{\parallel}$ (3.3) is a constant independent of R, $G_R^{\parallel}(z) = m_z^2$, where m_z is the magnetization per spin. When $K \to \infty$ ($K \to -\infty$) the system is frozen in the $|\uparrow\uparrow \cdots \uparrow\rangle$ ($|\downarrow\downarrow \cdots \downarrow\rangle$) state. The multicritical points (3.1)–(3.2) are in the same universality class as the $\gamma = 0$, $h = 1$, $\Delta = 0$ point of the XY model,[4] except for the KDP-like first-order transition point[20,31] at the isotropic Heisenberg point $\gamma = 0$, $h = 0$, $\Delta = 1$.

4. FURTHER APPLICATIONS OF THE PESCHEL–EMERY METHOD

The PE method can be generalized in two ways. One may start, for example, with more complicated models than (2.1) when constructing the L operator. Another possibility is to change the dynamic behavior by allowing for more simultaneous spin flips, or by enforcing different conservation laws.[12,14]

Our first example is the search for order lines in the dimerized (staggered) XYZ chain, which is an important model from both the experimental[6] and theoretical points of view.[31] One starts with the one-dimensional staggered Ising model:

$$-\beta H^{\text{eff}} = \sum_k (K_1 s_{2k} s_{2k+1} + K_2 s_{2k+1} s_{2k+2}) \tag{4.1}$$

Following the same steps as those leading to (2.13) one first chooses the transition probabilities as

$$\begin{aligned} w_{2k} &= \left(\frac{\alpha_0 + \alpha_1}{2} + \frac{\alpha_0 + \alpha_1}{2} s_{2k-1} s_{2k+1} \right) \exp(-s_{2k} h_{2k}) \\ w_{2k+1} &= \left(\frac{\beta_0 + \beta_1}{2} + \frac{\beta_0 - \beta_1}{2} s_{2k} s_{2k+2} \right) \exp(-s_{2k+1} h_{2k+1}) \end{aligned} \tag{4.2}$$

and after some algebraic manipulations one gets the dual of the Liouville operator as

$$L^D = \sum_k (L^D_{2k} + L^D_{2k+1}) \tag{4.3}$$

where

$$L^D_{2k} = A_1 \tau^z_{2k} \tau^z_{2k+1} + B_1 \tau^z_{2k} + C_1 \tau^x_{2k} \tau^x_{2k+1} - D_1 \tau^y_{2k} \tau^y_{2k+1} \tag{4.4a}$$

$$L^D_{2k+1} = A_2 \tau^z_{2k+1} \tau^z_{2k+2} + B_2 \tau^z_{2k+1} + C_2 \tau^x_{2k+1} \tau^x_{2k+2} - D_2 \tau^y_{2k+1} \tau^y_{2k+2}, \tag{4.4b}$$

and

$$\begin{aligned}
A_1 &= \frac{\alpha_0 - \alpha_1}{2} C^+ + \frac{\alpha_0 + \alpha_1}{2} C^-, \qquad A_2 = \frac{\beta_0 - \beta_1}{2} C^+ + \frac{\beta_0 + \beta_1}{2} C^- \\
B_{1,2} &= \left[\left(\frac{\alpha_0 - \alpha_1}{2} + \frac{\beta_0 - \beta_1}{2} \right) S^{\pm} + \left(\frac{\alpha_0 + \alpha_1}{2} + \frac{\beta_0 + \beta_1}{2} \right) S^{\mp} \right] \\
C_1 &= -\frac{\alpha_0 + \alpha_1}{2}, \qquad C_2 = -\frac{\beta_0 + \beta_1}{2}, \\
D_1 &= -\frac{\alpha_0 - \alpha_1}{2}, \qquad D_2 = -\frac{\beta_0 - \beta_1}{2} \\
C^{\pm} &= \tfrac{1}{2} \left[\cosh(K_2 + K_1) \pm \cosh(K_2 - K_1) \right] \\
S^{\pm} &= \tfrac{1}{2} \left[\sinh(K_2 + K_1) \pm \sinh(K_2 - K_2) \right]
\end{aligned} \tag{4.5}$$

This dual form of the Liouville operator should be compared to the Hamiltonian of the dimerized XYZ chain:

$$H^{\text{stagg}}_{XYZ} = -\sum_k \{ H_{2k} + 2h_1 \tau^z_{2k} + \tau H_{2k+1} + 2h_2 \tau^z_{2k+1} \} \tag{4.6}$$

where

$$H_j = (1 + \gamma) \tau^x_j \tau^x_{j+1} + (1 - \gamma) \tau^y_j \tau^y_{j+1} + \Delta \tau^z_j \tau^z_{j+1} \tag{4.7}$$

By matching the corresponding couplings of (4.3) and (4.6) and then eliminating α_0, α_1, β_0, β_1, K_1, and K_2 one obtains a rather complicated formula for the *order* surface of the dimerized Hamiltonian (4.6). The result for the free-fermion case $\Delta = 0$ is

$$(1 - \gamma^2)(1 + \tau)^2 = 4h_1 h_2 \tag{4.8}$$

The second example is related to the three-dimensional Ising model shown in Fig. 2. In this model hexagonal planes are connected by vertical nearest-neighbor ferromagnetic interactions. Within the hexagonal planes one has a ferromagnetic nearest neighbor interaction K_1, a next-to-nearest neighbor antiferromagnetic interaction, $-|K_2|$, and a four-spin coupling

$K_4 > 0$, as shown in Fig. 2b. At $T = 0$ the spins form ferromagnetic chains in the vertical direction, while within the hexagonal plane one has the basic configurations shown in Fig. 3. The emerging ordered phases and the $T = 0$ phase diagram are also shown. The hexagonal plane-to-hexagonal plane transfer matrix of this model can be written as

$$T = T_1 T_2 \tag{4.9}$$

where T_1 is the self-energy of a plane,

$$T_1 = \exp \sum_{\mathbf{r}} \left\{ k_1 \sum_{\alpha} \sigma^z_{\mathbf{r}} \sigma^z_{\mathbf{r},\alpha} - |K_2| \sum_{\alpha_1 \neq \alpha_2} \sigma^z_{\mathbf{r},\alpha_1} \sigma^z_{\mathbf{r},\alpha_2} + K_4 \sigma^z_{\mathbf{r}} \sigma^z_{\mathbf{r},1} \sigma^z_{\mathbf{r},2} \sigma^z_{\mathbf{r},3} \right\} \tag{4.10}$$

$\mathbf{r}$ runs over the lattice sites of the hexagonal lattice and $\alpha = 1, 2, 3$ over the nearest neighbors. T_2 represents the interaction between two planes and is

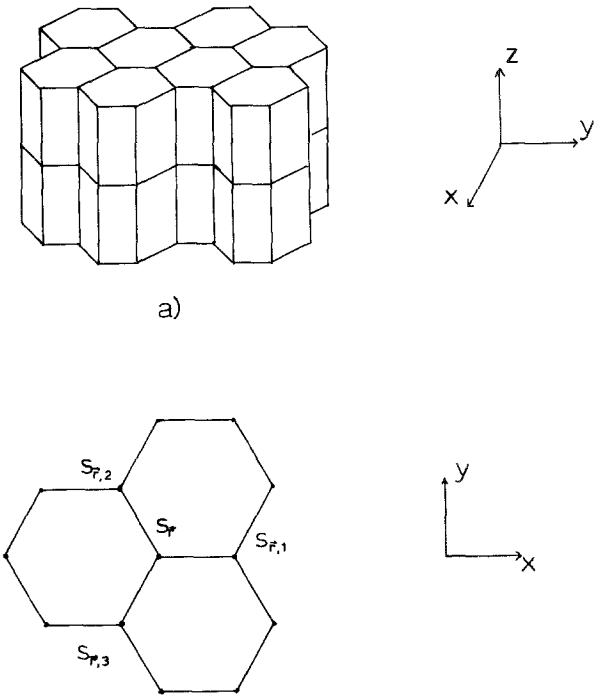

Fig. 2. The hexagonal Ising model with biaxial competing interactions within the hexagonal planes. The interaction between planes is ferromagnetic, $J_z < 0$. Within the planes (Fig. 2a) one has a ferromagnetic interaction ($J_1 < 0$) between the spin $s_{\mathbf{r}}$ and the nearest neighbors $s_{\mathbf{r},\alpha}$, $\alpha = 1, 2, 3$; an antiferromagnetic interaction ($J_2 > 0$) between spins $s_{\mathbf{r},\alpha_1}$ and $s_{\mathbf{r},\alpha_2}$ ($\alpha_1 \neq \alpha_2$) and a four-spin interaction $J_4 < 0$ between spins $s_{\mathbf{r}}$, $s_{\mathbf{r},1}$, $s_{\mathbf{r},2}$, and $s_{\mathbf{r},3}$.

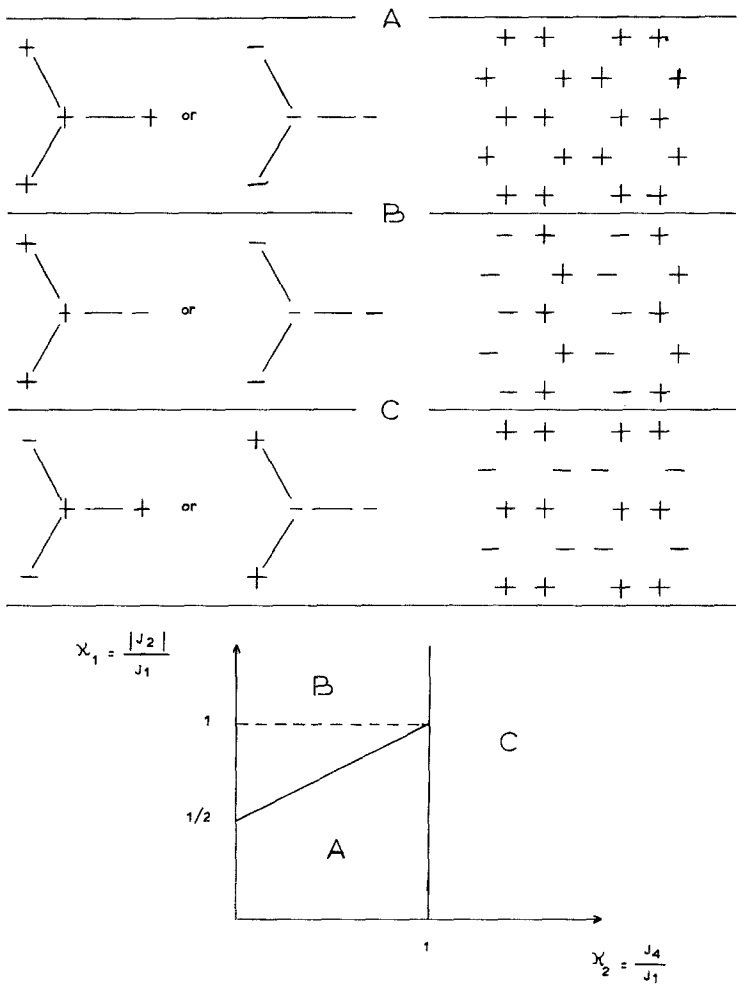

Fig. 3. The $T = 0$ possible ground states of the hexagonal Ising model with competing interactions. The different ordered phases are denoted by A, B, and C. The $T = 0$ phase diagram is also shown.

given by

$$T_2 = \text{const} \exp\left(K_z^* \sum_{\mathbf{r}} \sigma_{\mathbf{r}}^x \right) \tag{4.11}$$

where

$$K_z^* = -\tfrac{1}{2} \ln \tanh K_z \tag{4.12}$$

When taking the (Hamiltonian) limit $K_z^*, K_1, |K_2|, K_4 \to 0$ (but keeping constant the ratios $\kappa_1 = |K_2|/K_1$; $\kappa_2 = K_4/K_1$; $\tau = K_z^*/K_1$) one can expand the exponents in (4.10), (4.11), keep only the linear terms in couplings and

omit the constant term. What is left is a 1/2-spin Hamiltonian defined on a honeycomb lattice:

$$\hat{H} = -\sum_{\mathbf{r}} \left\{ \sum_{\alpha} \sigma_{\mathbf{r}}^z \sigma_{\mathbf{r},\alpha}^z - \kappa_1 \sum_{\alpha_1 \neq \alpha_2} \sigma_{\mathbf{r},\alpha_1}^z \sigma_{\mathbf{r},\alpha_2}^z + \kappa_2 \sigma_{\mathbf{r}}^z \sigma_{\mathbf{r},1}^z \sigma_{\mathbf{r},2}^z \sigma_{\mathbf{r},e}^z + \tau \sigma_{\mathbf{r}}^x \right\} \tag{4.13}$$

Next, consider a two-dimensional Ising model on a hexagonal lattice:

$$-\beta H^{\text{eff}} = K^{\text{eff}} \sum_{\mathbf{r},\alpha} s_{\mathbf{r}} s_{\mathbf{r},\alpha} \tag{4.14}$$

The corresponding Liouville operator is constructed through the same steps as before and choosing $f_{\mathbf{r}} = 1$, one gets

$$L = \sum_{\mathbf{r}} \left\{ A + B \sum_{\alpha_1 \neq \alpha_2} \sigma_{\mathbf{r},\alpha_1}^z \sigma_{\mathbf{r},\alpha_2}^z - C \sum_{\alpha} \sigma_{\mathbf{r}}^z \sigma_{\mathbf{r},\alpha}^z - D \sigma_{\mathbf{r}}^z \sigma_{\mathbf{r},1}^z \sigma_{\mathbf{r},2}^z \sigma_{\mathbf{r},3}^z - \sigma_{\mathbf{r}}^x \right\} \tag{4.15}$$

with

$$\begin{aligned} A &= \tfrac{1}{4}(\cosh 3K^{\text{eff}} + 3\cosh K^{\text{eff}}) \\ B &= \cosh K^{\text{eff}} \sinh^2 K^{\text{eff}} \\ C &= \sinh K^{\text{eff}} \cosh^2 K^{\text{eff}} \\ D &= \sinh^3 K^{\text{eff}} \end{aligned} \tag{4.16}$$

Matching the couplings of (4.13) to (4.15), (4.16) one obtains the trajectory given by

$$\kappa_1^2 = \kappa_2, \qquad \tau^2 = (1 - \kappa_2)^3 / \kappa_2 \tag{4.17}$$

By changing the temperature ($\sim\tau$) one moves on (4.17) from high temperatures to low temperatures until the point

$$\bar{\kappa}_1^2 = \bar{\kappa}_2 = \tanh^2 K_c^{\text{hex}} = \tfrac{1}{3} \tag{4.18}$$

where the two-dimensional hexagonal Ising model undergoes a phase transition. The critical exponents of $\xi_{\|}$ and $\xi_{\perp}$ are, respectively,

$$\nu_{\|} = 1$$

$$\nu_{\perp} = 2.125$$

Note that $\nu_{\perp}$ equals the dynamic critical exponent, z, of the two-dimensional kinetic Ising model.[32] Below the multicritical point (4.18) the ground state is doubly degenerate and one has an *order* line ending at $\tau = 0$ ($T = 0$) on the multicritical point $\kappa_1 = \kappa_2 = 1$ (see Fig. 3). It seems possible that this three-dimensional Ising model has an incommensurate (floating) phase. In that case the multicritical point (4.18) is a good candidate for being a multicritical Lifshitz point. It is also plausible that below τ_c (4.18) the order line (4.17) is lying on the ferromagnetic boundary.

5. DISCUSSION AND CONCLUSIONS

The Peschel–Emery method is an elegant and powerful method for determining the ground state and the ground state energy along disorder (order) trajectories in quantum spin systems at $T = 0$. Interesting enough, it suggests also a way to measure the dynamic critical exponent z from static measurements (through the relation $\nu_\perp = z \cdot \nu_\parallel$). It is clear that the very existence of these special trajectories is a result of the anisotropic competing interactions. The question is then whether this is a general feature of *all* such models or not? In order to discuss this basic question it is useful to consider the following one-dimensional Hamiltonian:

$$\hat{H}(q) = -\sum_j (\sigma_j^z \sigma_{j+1}^z - \kappa \sigma_j^z \sigma_{j+q}^z + \tau \sigma_j^x), \qquad q \geqslant 2 \tag{5.1}$$

For $q = 2$ this Hamiltonian represents a special limit of the row-to-row transfer matrix of the axial-next-nearest-neighbor Ising (ANNNI) model.[1,33] In general, the model (5.1) has a n.n. ferromagnetic interaction (the first term of the sum), competing with a qth-neighbor antiferromagnetic interaction (the second term). The last term of (5.1) plays the role of the temperature operator. For $q = 2$ (ANNNI model) Peschel and Emery have demonstrated the presence of a disorder line.[1] [This line is the intersection of the (2.17) surface with the plane $\gamma = 1$.] For $q = 3$, however, the $\hat{H}(q = 3)$ operator (5.1) cannot be mapped into the time evolution operator of the Ising model (2.1), no matter what the prescribed dynamics might be. In other words, the PE method does not work for $\hat{H}(3)$. A more general definition of the $\bar{\kappa}(\tau)$ disorder trajectory can be given as

$$\xi^{\parallel}(\bar{\kappa}, \tau) = \text{minimum} \qquad (\tau \text{ fixed}) \tag{5.2}$$

independently of the fact whether the ground state energy of (5.1) can or cannot be exactly calculated on $\bar{\kappa}(\tau)$. I suggest that the models exhibiting disorder (order) trajectories have the following properties:

(A) When changing the competition ratio κ at fixed (high) temperature τ the spin–spin correlation function along the competition axis is exponentially decaying for $\kappa < \bar{\kappa}(\tau)$ but is modulated by a (κ, τ)-dependent wave vector for $\kappa > \bar{\kappa}(\tau)$. This change should be detectable in experiments for Monte Carlo simulations and should *not* be confused to a disorder-incommensurate phase transition.

(B) The minimum of $\xi^{\parallel}$ is related to the crossing of the second and the third largest eigenvalues of a corresponding transfer matrix (see next paper). In general one should expect the same cusplike minimum as in the triangular Ising model,[2] involving a nonanalytical behavior on $\bar{\kappa}(\tau)$.[2,4] This fact explains the poor convergence of the high-temperature expansions

in the ANNNI Hamiltonian $H(q = 2)$ (5.1).[33] It shows that one must be very cautious when using exact series expansions to determine phase boundaries in systems with competing interactions.

(C) Usually the $\bar{\kappa}(\tau)$ line should end on a multicritical point with a strong anisotropic character (see Section 3).

(D) In some cases the ground state energy of the model can be exactly calculated on $\bar{\kappa}(\tau)$. If this is not the case, approximate methods can be used to determine $\bar{\kappa}(\tau)$.[34]

Finally, let me remark that the Peschel–Emery method works only for *quantum*-spin Hamiltonians. Since in many cases these Hamiltonians are rigorously or approximately related to the transfer matrix of higher-dimensional *classical* spin systems one may ask if it is possible to find order and disorder trajectories in such models. The answer is positive and is detailed in the second paper.

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REFERENCES

1. I. Peschel and V. J. Emery, *Z. Phys. B* **43**:241 (1981). For a different approach see also J. Kurman, H. Thomas, and G. Müller, *Physica A*, to be published.
2. J. Stevenson, *Can. J. Phys.* **48**:2118 (1970); *J. Math. Phys.* **11**:420 (1970).
3. M. B. Geilikmann, *Sov. Phys. JETP* **39**:570 (1974); E. Fradkin and T. P. Eggarter, *Phys. Rev. A* **14**:495 (1976).
4. E. Barouch and B. McCoy, *Phys. Rev. A* **3**:786 (1971).
5. M. Steiner, J. Villain, and G. G. Windsor, *Adv. Phys.* **25**:87 (1976).
6. J. C. Bonner, H. W. J. Blöte, H. Beck, and G. Müller, in *Physics in One Dimension*, J. Bernasconi and T. Schneider, eds., Springer-Verlag, New York (1981).
7. J. T. Devreese, R. P. Evrard, and V. E. van Doren, eds., *Highly Conducting One-Dimensional Solids*, Plenum Press, New York (1980).
8. B. Sutherland, *J. Math. Phys.* **11**:3183 (1970).
9. R. J. Baxter, *Ann. Phys. (N.Y.)* **70**:193, 323 (1972).
10. E. Fradkin and L. Susskind, *Phys. Rev. D* **17**:2637 (1978).
11. For a review see P. W. Kasteleyn, in *Fundamental Problems in Statistical Mechanics*, Vol. 3, E. D. G. Cohen, ed., North-Holland, Amsterdam (1975).
12. For a recent review see P. C. Hohenberg and B. I. Halperin, *Rev. Mod. Phys.* **49**:435 (1977).
13. R. Glauber, *J. Math. Phys.* **4**:294 (1963).
14. See K. Kawasaki, in *Phase Transitions and Critical Phenomena*, Vol. II, C. Domb and M. S. Green, eds., Academic, New York (1972).

15. B. U. Felderhof, *Rep. Math. Phys.* **1**:215 (1970); E. D. Siggia, *Phys. Rev. B* **16**:2319 (1977).
16. H. A. Kramers and G. H. Wannier, *Phys. Rev.* **60**:252 (1941); L. Mittag and M. J. Stephen, *J. Math. Phys.* **12**:441 (1971).
17. R. J. Baxter, *Ann. Phys. (N.Y.)* **76**(1), 25, 48 (1973).
18. J. D. Johnson, S. Krinski, and B. M. McCoy, *Phys. Rev. A* **8**:2526 (1973).
19. B. M. McCoy and T. T. Wu, *Nuovo Cimento* **56B**:311 (1968).
20. C. N. Yang and C. P. Yang, *Phys. Rev.* **150**:321 (1966).
21. J. D. Johnson and B. M. McCoy, *Phys. Rev. A* **4**:1613 (1972).
22. E. Lieb, T. Schultz, and D. Mattis, *Ann. Phys. (N.Y.)* **16**:407 (1961).
23. S. Katsura, *Phys. Rev.* **127**:1508 (1962).
24. T. Niemeijer, *Physica* **36**:377 (1967).
25. M. Suzuki, *Progr. Theor. Phys.* **46**:1377 (1971).
26. M. J. Stephen and L. Mittag, *J. Math. Phys.* **13**:1944 (1972).
27. W. Selke and M. E. Fisher, *Z. Phys. B* **40**:71 (1980).
28. S. Redner, *J. Stat. Phys.* **25**:15 (1981).
29. F. Haake and K. Thol, *Z. Phys. B* **40**:219 (1980); R. Pandit, G. Forgács, and P. Ruján, *Phys. Rev. B* **24**:1576 (1981).
30. R. M. Hornreich, R. Liebman, H. G. Schuster, and W. Selke, *Z. Phys. B* **35**:91 (1979).
31. For a review of ferroelectric models see E. H. Lieb and F. Y. Wu, in *Phase Transitions and Critical Phenomena*, Vol. II, C. Domb and M. S. Green, eds., Academic Press, London (1972); J. L. Black and V. J. Emery, *Phys. Rev. B* **23**:429 (1981); M. Kohmoto, M. P. M. den Nijs, and L. P. Kandanoff, *Phys. Rev. B* **24**:5229 (1981); C. J. Hamer, *J. Phys. A* **14**:2981 (1981).
32. Z. Rácz and M. F. Collins, *Phys. Rev. B* **13**:3074 (1973).
33. P. Ruján, *Phys. Rev. B* **24**:6620 (1981); M. N. Barber and P. M. Duxbury, *J. Phys. A* **14**:L251 (1981).
34. P. Ruján, in preparation.