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The Ising model in a transverse field on comb-like ramified linear structures

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Résumé. — En utilisant à la fois une méthode de renormalisation et des résultats exacts, le modèle d'Ising dans un champ transverse a pu être étudié à $T = 0$ pour des réseaux linéaires ramifiés en forme de peigne.

Abstract. — Combining a real space renormalization group method and exact results, the Ising model with a transverse field has been studied at $T = 0$ for comb-like ramified linear structures.

The Ising model with a transverse field described by the Hamiltonian

$$\mathcal{H} = -J \sum_{ij} S_i^x S_j^x - \Gamma \sum_i S_i^z, \quad (1)$$

where S_i^x , S_i^y , S_i^z are Pauli spin 1/2 matrices, provides a good representation for physical systems having constituents with two low-lying energy levels which can be sponsored by states $S_i^z = \pm 1$. These include for instance phase transitions in magnetic materials with a pair of singlet crystal field levels [1] and in hydrogen-bonded ferroelectrics [2].

This model has been extensively studied when the sites i, j are nearest neighbours on a regular D dimensional lattice [3], [4]. In one dimension ($D = 1$) the model can be solved exactly [5]. In higher dimensions only approximate calculations exist at the moment either from series expansions [6] or from real space renormalization group methods [7], [8]. At finite temperature $T \neq 0$ this quantum model behaves similarly to the classical Ising model and spontaneous order appears below a critical temperature $T_c(\Gamma)$ which is non zero for $D \geq 2$. At low temperature ($T \rightarrow 0$) quantum effects show up. At $T = 0$ a new behaviour is expected. At $T = 0$ when the transverse field Γ varies the ground state displays a second order phase transition. For Γ/J less than a critical value $(\Gamma/J)_c$ the ground state $|0\rangle$ is asymptotically (in the limit of an infinite system) doubly degenerate with a spontaneous

order parameter $M^x = \langle 0 | S_i^x | 0 \rangle$; for Γ/J larger than $(\Gamma/J)_c$ the ground state becomes non-degenerate and the order disappears. This transition exists for $D \geq 1$. For $D = 1$ the critical field is equal to 1 [5] (duality exists) and the exact solution maps onto the Onsager exact solution [9] for the $D = 2$ classical Ising model (at finite temperature). This analogy extends to D dimensions as shown by Suzuki [10]: the D -dimensional Ising model in a transverse field at $T = 0$ is equivalent to a $D + 1$ dimensional classical Ising model ($\Gamma = 0$) at $T \neq 0$ (the transverse field plays the role of a temperature).

The dilute Ising model in a transverse field has also been considered [11], [12]. It is related to phase transitions in a number of dilute systems [13]. The model is defined as follows: the sites i, j are defined on a regular periodic lattice but a proportion p of the sites are missing (the non-dilute model corresponds to $p = 0$). At $T = 0$ for $D \geq 2$ when the concentration p of non-magnetic sites increases the critical transverse field $(\Gamma/J)_c(p)$ goes down and when p is larger than the percolation threshold p_c (p_c depends on the lattice considered; for instance for a cubic lattice $p_c \simeq 0.693$), there is no more infinite cluster and no ordered ground state exists leading to $(\Gamma/J)_c(p) = 0$ for $p > p_c$. It has been argued [11] that at $p = p_c$ the critical field $(\Gamma/J)_c(p_c)$ is not zero and is larger than 1, the value for the linear chain. This is due to the fact that the Ising model in a transverse field has always a transition if the lattice structure (regular or not) is infinite and if, due to inequalities for spin quantum systems [14], $(\Gamma/J)_c$ increases when new bonds are added. This situation is different from the usual dilute classical Ising model [15] where $T_c(p)$ goes continuous-

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ly to zero (for classical Ising models there is no ordered phase on a linear chain) as shown in recent experiments [16]. For the dilute transverse field Ising model, the critical field $(\Gamma/J)_c$ ($p = p_c$) reflects the detailed structure of the infinite percolating cluster (concentration of free ends, loops, dead ends... etc.). This critical field can be in principle evaluated (up to now series expansions have failed to give a definite answer [12] but real space renormalization group methods are presently used in this perspective). To relate $(\Gamma/J)_c$ ($p = p_c$) to the structure of the cluster it is necessary to understand how the structure affects the critical field. This is partially achieved in this letter where we show how one can study a quantum model on a ramified lattice. We shall consider here a regular ramified lattice but as shown later the method can be extended to more general non regular structures.

The method consists in using first a block real-space renormalization-group iteration scheme introduced for quantum systems at $T = 0$ [17], [18] and the Hamiltonian (1) on a ramified linear structure is reduced to a similar Hamiltonian with new parameters on a linear chain which then is solved exactly using results of ref. [5]. This will be illustrated with simple comb-like structures.

Let us first study the comb structure shown in figure 1. The Hamiltonian (1) defined on such an infinite translationally invariant lattice is divided into inter- and intra-block parts (the blocks are made of six sites labelled from 1 to 6). The transverse field Ising model is solved exactly for the block part and the two lowest levels $|+\rangle$ and $|-\rangle$ with energies E_+ and E_- are retained. A new set of spin 1/2 operators $S^{x'}$ is associated with each block (the eigenstates of $S^{z'}$ are $|+\rangle$ and $|-\rangle$) and the intra-block parts are rewritten in the new spin representations. Taking the matrix elements of the old spins $S_{j,p}$ (j being the label of the block and p the label of the spin in the block) between the block states $|+\rangle$ and $|-\rangle$ we get the relation (see reference [18])

$$S_{j,p}^x = \xi_p^x S_j^x.$$

(2)

Fig. 1. — An example of block partitioning in the case $C = 1$.

Table I. — *Summary of the results. For each different ramified structure studied (corresponding to different concentrations C of free ends) and each block used in the partitioning method, the result for $(\Gamma/J)_c$ is given and the corresponding label in figure 1 is precised.*

System _i	C	block	$(\Gamma/J)_c$	Symbol
	$1/7 = 0.142\ 8$		1.073	○
	$1/3 = 0.333\ 3$		1.144	○
			1.138	●
	$1/2 = 0.5$		1.178	○
			1.194	●
	$2/3 = 0.666\ 7$		1.256	○
			1.227	●
	1.		1.098	
			1.294	○
			1.307'	●
			1.300	×

The inter-block interaction is rewritten as a function of the new spin operators and $\mathcal{H}$ is replaced by $\mathcal{H}'$ which has the same form eq. (1) with an extra constant term C' and with new parameters Γ' and J' . The ground state of $\mathcal{H}(\Gamma, J)$ is thus directly related to the ground state of $\mathcal{H}'(\Gamma', J', C')$ which is defined on a linear chain of the new block spins and can be solved exactly. From the recursion relations we get

$$\frac{\Gamma'}{J'} = f(\Gamma/J) \quad (3)$$

and then

$$\left(\frac{\Gamma}{J}\right)_c = f^{-1}\left(\frac{\Gamma'}{J'} = 1\right). \quad (4)$$

We have a certain freedom in choosing the block partitioning. The method is asymptotically exact (we tend to the exact results when the size of the blocks increases).

The method has been used for several comb-like structures. Different blocks have been used. The results for $(\Gamma/J)_c$ are shown in table I. Physical quantities at $T = 0$ can also be calculated. For instance we can determine the order parameter $M_i^x = \langle 0 | S_i^x | 0 \rangle$ which is non zero for $\Gamma/J < (\Gamma/J)_c$. There are now two possible order parameters which go to zero at the same time in the same way. Either M_b^x corresponding to a site in the backbone of the comb or M_e^x at a free end of the comb. Using eq. (2), eq. (3) and the results of ref. [5], we get for the comb of figure 1

$$\left. \begin{aligned} M_b^x &= \xi_2^x(\Gamma/J) \cdot (1 - f^2(\Gamma/J))^{1/8} \\ M_e^x &= \xi_5^x(\Gamma/J) \cdot (1 - f^2(\Gamma/J))^{1/8} \end{aligned} \right\} \quad (5)$$

These magnetizations are plotted in figure 2. We check that due to free-end effects $M_e^x < M_b^x$ but close to $(\Gamma/J)_c$ they both go to zero with the same power law. The other comb structures studied (table I) correspond to several values of

$$C = \frac{\text{number of free ends}}{\text{number of backbone sites}}$$

where C varies from 0 to 1 ($C = 0, 1/7, 1/2, 2/3, 1$). The results for $(\Gamma/J)_c$ as a function of C are plotted in figure 3.

The next step shall be to explore more complicated regular and non-regular ramified structures. For regular structures we can introduce longer and more

Fig. 2. — Results for the magnetizations M_e^x (free end site) and M_b^x (backbone site) as the function of Γ/J calculated for $C = 1$ with the blocks represented in figure 1.

Fig. 3. — Results for $(\Gamma/J)_c$ plotted as a function of C .

complicated side chains, loops, etc... For non-regular structures the same method applies but the new Hamiltonian $\mathcal{H}'$ is defined on a linear chain with different Γ_i and $J_{i,i+1}$. For such a model a complete solution does not exist at the moment but the critical point is given by [19]

$$\prod_{i=1}^{\infty} \Gamma_i = \prod_{i=1}^{\infty} J_{i,i+1}. \quad (6)$$

Finally, the method presented here can be applied to other quantum systems and can be also used to study large finite size systems.

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