Phase transitions of the mixed spin-1/2 and spin-S Ising model on a three-dimensional decorated lattice with a layered structure ⋆

Jozef Strečka, Lucia Čanová, and Ján Dely

Department of Theoretical Physics and Astrophysics, Faculty of Science, P. J. Šafárik University, Park Angelinum 9, 040 01 Košice, Slovak Republic

Abstract

Phase transitions of the mixed spin-1/2 and spin-S ($S \geq 1$) Ising model on a three-dimensional (3D) decorated lattice with a layered magnetic structure are investigated within the framework of a precise mapping relationship to the simple spin-1/2 Ising model on the tetragonal lattice. This mapping correspondence gives for the layered Ising model of mixed spins accurate analytical results when taking into account two recent conjectures on the exact solution of the spin-1/2 Ising model on the orthorhombic lattice [Z.-D. Zhang, Phil. Mag. 87 (2007) 5309-5419]. It is shown that the critical behaviour markedly depends on a relative strength of axial zero-field splitting parameter, inter- and intra-layer interactions. The striking spontaneous order captured to the 'quasi-1D' spin system is found in a restricted region of interaction parameters, where the zero-field splitting parameter forces all integer-valued decorating spins towards their 'non-magnetic' spin state.

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1 Introduction

Phase transitions and critical phenomena of rigorously solvable interacting many-particle systems are much sought after in the modern equilibrium statis-

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Email address: `jozef.strecka@upjs.sk` (Jozef Strečka).
URL: `http://158.197.33.91/~strecka` (Jozef Strečka).

tical mechanics as they offer valuable insight into a cooperative nature of phase changes [1]. Beside this, the usefulness of mathematically tractable models can also be viewed in providing guidance on a reliability of various approximative techniques, which are often needed for treating more complicated models that preclude exact analytical treatment. *Decorated planar Ising models*, which can be constructed by adding one or more spins on bonds of some original lattice, belong to the simplest mathematically tractable lattice-statistical models (see Ref. [2] and references cited therein). The main advantage of decorated planar Ising models consists in a relative ease of obtaining their exact solutions. As a matter of fact, several decorated planar Ising models can straightforwardly be solved by employing the generalized decoration-iteration transformation [3] that relates their exact solution to that one of the simple spin-1/2 Ising model on a corresponding (undecorated) lattice, which is generally known for many planar lattices of different topologies [4,5,6].

Quite recently, the decorated Ising models consisting of mixed spins have attracted a great deal of attention on account of much richer critical behaviour in comparison with their single-spin counterparts. Exact solutions of the mixed-spin Ising models on several decorated planar lattices have furnished a deeper insight into diverse attractive issues of statistical mechanics such as multiply reentrant phase transitions [7,8,9,10,11,12,13], multicompensation phenomenon [11,12,13,14], annealed disorder [15,16,17,18,19,20], as well as, the effect of non-zero external magnetic field [21,22,23]. In addition, the mixed-spin Ising models on some decorated planar lattices can also be viewed as useful model systems for some ferromagnetic, ferrimagnetic, and metamagnetic molecular-based magnetic materials (see Refs. [24,25] for excellent recent reviews).

Among the most convenient properties of the generalized decoration-iteration transformation one could mention its general validity, which means that this mapping transformation holds independently of the lattice spatial dimension to be considered. Unfortunately, the application of decoration-iteration mapping was until lately basically restricted to one- and two-dimensional decorated lattices due to the lack of the exact solution of the spin-1/2 Ising model on three-dimensional (3D) lattices. The majority of studies concerned with the mixed-spin Ising models on 3D decorated lattices were therefore based on approximative analytical methods such as mean-field and effective-field theories [26,27,28,29,30,31,32]. On the other hand, essentially exact results were recently reported by Oitmaa and Zheng [33] for phase diagrams of the mixed-spin Ising model on the decorated cubic lattice by adopting the decoration-iteration transformation and the critical temperature of the corresponding spin-1/2 Ising model on the simple cubic lattice, which is known with a high numerical precision from the high-temperature series expansion [34]. Another possibility of how rather accurate results can be obtained for the mixed-spin Ising model on 3D decorated lattices is to perform extensive Monte-Carlo simulation as recently done by Boughrara and Kerouad for the decorated Ising film [35].

In the present work, the mixed spin-1/2 and spin-S Ising model on the layered 3D decorated lattice will be studied in particular by applying the decoration-iteration transformation and adopting two recent conjectures on the exact solution of the spin-1/2 Ising model on the orthorhombic lattice [36]. Even although there still might be a controversial debate about correctness of both Zhang's conjectures [36], the critical point as well as other thermodynamic quantities seem to be in a reasonable accordance with precise numerical estimates of other accurate numerical methods [36,37]. From this point of view, one should expect just small numerical error (if any) even if the conjectured exact solution will finally turn out to be erroneous. Owing to this fact, the combination of the generalized decoration-iteration transformation [3] with Zhang's putative exact solution [36] might give rather accurate results and the main advantage of this combination is that it preserves the analytic form of the solution to be obtained for the layered mixed-spin Ising model.

The outline of this paper is as follows. In Section 2, the detailed description of the layered Ising model of mixed spins is presented at first. Then, some details of the decoration-iteration mapping are clarified along with the derivation of exact expressions for the magnetization and critical temperatures. The most interesting results are presented and detailed discussed in Section 3. Finally, some concluding remarks are mentioned in Section 4.

2 Ising model and its solution

Let us define the mixed spin-1/2 and spin-S ($S \geq 1$) Ising model on the layered 3D decorated lattice as it is diagrammatically depicted in Fig. 1. In this figure, the solid circles denote lattice positions of the spin-1/2 Ising atoms that reside sites of the simple cubic lattice and the empty ones represent lattice positions of the decorating spin-S Ising atoms lying on each bond of the simple cubic lattice. Let us further denote the total number of layers by the symbol N_L and the total number of the spin-1/2 atoms within each layer by the symbol N. The model under investigation can be then defined through the Hamiltonian

$$H = -J \sum_{l=1}^{N_L} \sum_{(i,j)}^{4N} S_{l,i} \sigma_{l,j} - J' \sum_{l=1}^{N_L} \sum_{j=1}^{N} \sigma_{l,j} \sigma_{l+1,j} - D \sum_{l=1}^{N_L} \sum_{i=1}^{2N} S_{l,i}^2, \tag{1}$$

where $\sigma_{l,j} = \pm 1/2$ and $S_{l,i} = -S, -S+1, \ldots, +S$ are two different kinds of Ising spins located in the lth layer at jth and ith lattice position, respectively. The parameter J denotes the intra-layer interaction between the nearest-

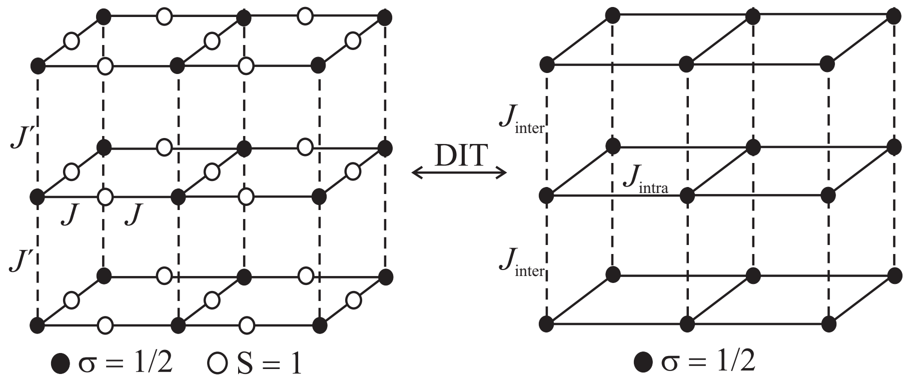

Fig. 1. Schematic representation of the mixed spin-1/2 and spin-S Ising model on the layered 3D decorated lattice and of its decoration-iteration transformation towards the simple spin-1/2 Ising model on the tetragonal lattice. Solid (empty) circles denote lattice positions of the spin-1/2 (spin-S) atoms, while solid and broken lines represent intra- and inter-layer interactions for both mixed-spin as well as effective spin-1/2 Ising model, respectively.

neighbour spin-1/2 and spin-S atoms, the parameter J' labels the inter-layer interaction between the nearest-neighbour spin-1/2 atoms from two adjacent layers and the parameter D stands for axial zero-field splitting (AZFS) parameter that acts on the decorating spin-S atoms only [38,39].

The partition function of the layered mixed-spin Ising model, which is defined through the Hamiltonian (1), can be written after straightforward rearrangement of some terms in the form

$$Z = \sum_{\{\sigma_{l,j}\}} \exp\left(\beta J' \sum_{l=1}^{N_L} \sum_{j=1}^{N} \sigma_{l,j}\sigma_{l+1,j}\right) \times \prod_{l=1}^{N_L} \prod_{i=1}^{2N} \sum_{S_{l,i}=-S}^{S} \exp\left[\beta J S_{l,i}\left(\sigma_{l,i1}+\sigma_{l,i2}\right) + \beta D S_{l,i}^2\right], \qquad (2)$$

where $\beta = 1/(k_\mathrm{B}T)$, k_B is Boltzmann's constant, T is the absolute temperature and the symbol $\sum_{\{\sigma_{l,j}\}}$ stands for a summation over all possible spin configurations of the spin-1/2 atoms. It can be readily seen from the structure of the relation (2) that the summation over spin degrees of freedom of the decorating spin-S atoms can be performed independently of each other (there is no direct interaction between the decorating spins) and before summing over all possible spin configurations of the spin-1/2 atoms. Both these facts enable us to introduce the generalized decoration-iteration transformation [2,3]

$$\sum_{S_{l,i}=-S}^{S} \exp[\beta J S_{l,i}(\sigma_{l,i1}+\sigma_{l,i2}) + \beta D S_{l,i}^2] = A \exp(\beta J_\mathrm{intra}\sigma_{l,i1}\sigma_{l,i2}), \qquad (3)$$

which effectively replaces all the interaction terms associated with the decorating spin $S_{l,i}$ and substitutes them by the equivalent expression that depends solely on its two nearest-neighbour vertex spins $\sigma_{l,i1}$ and $\sigma_{l,i2}$. Of course, the decoration-iteration transformation must retain its validity regardless of possible spin states of both the nearest-neighbour vertex spins $\sigma_{l,i1}$ and $\sigma_{l,i2}$ and this "self-consistency" condition unambiguously determines until now not specified transformation parameters A and $J_{\rm intra}$

$$A = \left\{ \left[\sum_{n=-S}^{S} \exp(\beta D n^2) \cosh(\beta J n) \right] \left[\sum_{n=-S}^{S} \exp(\beta D n^2) \right] \right\}^{1/2}, \qquad (4)$$

$$\beta J_{\rm intra} = 2 \ln \left[\sum_{n=-S}^{S} \exp(\beta D n^2) \cosh(\beta J n) \right] - 2 \ln \left[\sum_{n=-S}^{S} \exp(\beta D n^2) \right]. \qquad (5)$$

At this stage, the substitution of the decoration-iteration transformation (3) into Eq. (2) yields, after straightforward re-arrangement of few terms, the following mapping relationship for the partition functions

$$Z(\beta, J, J', D) = A^{2NN_L} Z_{\rm tetragonal}(\beta, J_{\rm intra}, J_{\rm inter} = J'). \qquad (6)$$

It is quite obvious that the mapping relation (6) relates the partition function of the layered Ising model on 3D decorated lattice to that one of the corresponding spin-1/2 Ising model on the tetragonal lattice (see Fig. 1). Notice furthermore that the effective intra-layer interaction $J_{\rm intra}$ of the corresponding spin-1/2 Ising model on the tetragonal lattice is temperature dependent parameter satisfying the self-consistency condition (5), while the effective inter-layer interaction $J_{\rm inter}$ is temperature independent parameter that is directly equal to the interaction parameter J'.

A calculation of the spontaneous magnetization and other thermodynamic quantities can be now accomplished in an easy and rather straightforward way. Adopting the mapping theorems developed by Barry *et al.* [40,41,42,43], the sublattice magnetization $m_{\rm A}$ relevant to the spin-1/2 atoms of the mixed-spin Ising model on 3D decorated lattice directly equals to the magnetization of the corresponding spin-1/2 Ising model on the tetragonal lattice

$$m_{\rm A}(\beta, J, J', D) \equiv \langle \sigma_{l,i} \rangle_{\rm decorated} = \langle \sigma_{l,i} \rangle_{\rm tetragonal} \equiv m_0(\beta, J_{\rm intra}, J_{\rm inter}). \qquad (7)$$

Above, the symbols $\langle \ldots \rangle_{\rm decorated}$ and $\langle \ldots \rangle_{\rm tetragonal}$ denote canonical ensemble averaging performed within the mixed-spin Ising model on the 3D decorated lattice and its corresponding spin-1/2 Ising model on the tetragonal lattice, respectively. On the other hand, the sublattice magnetization $m_{\rm B}$ of the spin-S atoms can easily be calculated by combining the exact Callen-Suzuki spin identity [44,45] with the differential operator technique [46,47]. It is noteworthy that this kind of mathematical treatment essentially follows Kaneyoshi's procedure [48] originally developed for the decorated planar Ising models, which connects the sublattice magnetization of the spin-S atoms with that one of the spin-1/2 atoms through the relation

$$m_{\rm B} \equiv \langle S_{l,i} \rangle_{\rm decorated} = 2 m_{\rm A} \frac{\sum\limits_{n=-S}^{S} n \exp(\beta D n^2) \sinh(\beta J n)}{\sum\limits_{n=-S}^{S} \exp(\beta D n^2) \cosh(\beta J n)}. \tag{8}$$

To complete our calculation of both sublattice magnetization, it is now sufficient to quote the analytic expression for the spontaneous magnetization of the corresponding spin-1/2 Ising model on the tetragonal lattice, which can be easily descended from Zhang's putative exact solution for the spin-1/2 Ising model on the orthorhombic lattice [36]

$$m_0 = \frac{1}{2} \left[\frac{(1 - x^2 - x^2 y^4 + x^4 y^4)^2 - 16 x^4 y^4}{(1 - x^2)^2 (1 - x^2 y^4)^2} \right]^{3/8}, \tag{9}$$

where $x = \exp(-\beta J_{\rm intra}/2)$ and $y = \exp(-\beta J_{\rm inter}/2)$. If both sublattice magnetization are known, the total magnetization of the mixed-spin Ising model on a 3D decorated lattice is given by the definition $m = (m_{\rm A} + 2 m_{\rm B})/3$.

Finally, let us conclude our calculation by specifying the critical condition that thoroughly determines a critical point of the order-disorder phase transition of the layered Ising model on 3D decorated lattice. It can be readily understood that both sublattice magnetization $m_{\rm A}$ and $m_{\rm B}$ tend necessarily to zero if the spontaneous magnetization m_0 of the corresponding spin-1/2 Ising model on the tetragonal lattice vanishes as well. Accordingly, the critical condition that enables to locate the order-disorder phase transition of the mixed-spin Ising model on 3D decorated lattice can also be readily found from Zhang's critical condition for the spin-1/2 Ising model on the orthorhombic lattice [36], which contains as a particular case the following critical condition for the spin-1/2 Ising model on the tetragonal lattice

$$\sinh\left(\frac{\beta_c J_{\rm intra}}{2}\right) \sinh\left(\frac{\beta_c J_{\rm intra}}{2} + \beta_c J_{\rm inter}\right) = 1, \tag{10}$$

where $\beta_c = 1/(k_{\rm B} T_c)$ and T_c denotes the critical temperature. It should be nevertheless mentioned that the above critical condition thoroughly determines a critical behaviour of the layered Ising model of mixed spins on assumption that the effective intra-layer interaction $J_{\rm intra}$ satisfies the mapping relation (5) and the effective inter-layer interaction is equal to $J_{\rm inter} = J'$.

3 Results and discussion

In this part, let us proceed to a discussion of the most interesting results obtained for the layered Ising model on 3D decorated lattice. Before doing this, it is worthy to mention that all analytical results presented in the preceding section are rather general as they hold for arbitrary quantum spin number S of the decorating spins and also independently of whether ferromagnetic or antiferromagnetic interactions J and J' are assumed. In what follows, we will restrict ourselves for simplicity just to an analysis of one particular example of the layered Ising model by considering both ferromagnetic interaction constants $J > 0$, $J' > 0$, and the special spin value $S = 1$. It is worthwhile to remark, however, that the qualitatively same behaviour might be expected for the layered Ising models with other integer values of the decorating spins as well. Besides, the presented zero-field phase diagrams should remain valid also for layered Ising models with the antiferromagnetic interaction(s) J and/or J' due to an invariance of Ising spin systems with respect to $J \to -J$ and $J' \to -J'$ interchange that merely causes a rather trivial change of the ferromagnetic ($J > 0, J' > 0$) alignment to the metamagnetic ($J > 0, J' < 0$), the ferrimagnetic ($J < 0, J' > 0$), or the antiferromagnetic ($J < 0, J' < 0$) one.

Let us begin our discussion by considering possible spin arrangements emerging in the ground state. It turns out that three different phases may appear in total at the zero temperature in dependence on a relative strength of the intra-layer interaction J, the inter-layer interaction J', and the axial zero-field splitting parameter D. The AZFS term D plays the role of the anisotropy parameter that forces all decorating spins $S = 1$ towards their 'non-magnetic' spin state $S_{l,i} = 0$ provided that this parameter is a sufficiently large negative number. The usual ferromagnetic phase (FP), which can be characterized through the following spin states of the decorating and vertex spins $(S_{l,i}; \sigma_{l,i}) = (1; 1/2)$, consequently represents the lowest-energy state just if $D/J > -1$. On the other hand, the striking 'quasi-1D' ferromagnetic phase (QFP) constitutes the ground state in a range of intermediate strong anisotropy parameters $D/J \in (-1 - J'/J, -1)$, where it exhibits an outstanding spontaneous long-range order unambiguously determined through the spin states $(S_{l,i}; \sigma_{l,i}) = (0; 1/2)$. The absence of any spontaneous long-range order can finally be detected in the disordered phase (DP), which is the lowest-energy state on assumption that $D/J < -1 - J'/J$. In this particular case, the sufficiently strong (negative) AZFS parameter energetically favours the 'non-magnetic' spin state $S_{l,i} = 0$ of the decorating spins and hence, there appears the spin state $(S_{l,i}; \sigma_{l,i}) = (0; \pm 1/2)$ with a complete randomness in the states of the vertex spins (the vertex spins from the same layer do not effectively feel each other). The most surprising finding stemming from the study of the ground state is a pure existence of QFP, which exhibits a remarkable spontaneous long-range order in spite of the 'non-magnetic' nature of the

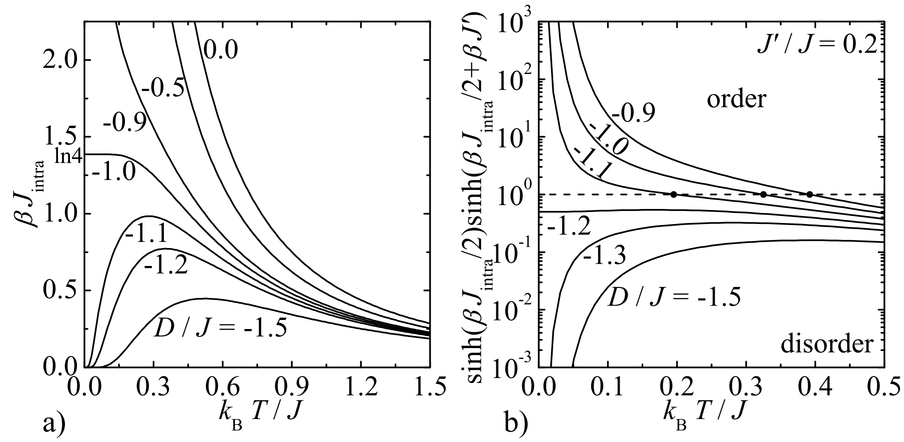

Fig. 2. Typical temperature dependences of the effective intra-layer coupling $\beta J_{\rm intra}$ obtained for several values of the anisotropy parameter D/J (Fig. 2a). Note that $\beta J_{\rm intra}$ is given by the mapping relation (5) and it does not depend on a strength of the inter-layer interaction J'. Fig. 2b) displays in a semi-logarithmic scale a graphical solution of the critical condition (10). Solid (broken) lines depict temperature dependences of the left-hand-side (right-hand-side) of the critical condition (10) for several values of the parameter D/J and the ratio $J'/J = 0.2$. The points of intersection between broken and solid lines (full circles) determine critical points.

decorating spins and the effectively 'quasi-1D' character of the spin system.

To provide a deeper insight into the mechanism that drives the spin system into one of those three available spin states, it might be useful to take a closer look at the effective coupling parameters $\beta J_{\rm intra}$ and $\beta J_{\rm inter}$ of the corresponding spin-1/2 Ising model on the tetragonal lattice. The effective inter-layer coupling $\beta J_{\rm inter} = J'/(k_{\rm B}T)$ is evidently monotonously decreasing function of the temperature, which diverges as T^{-1} when approaching the zero temperature. By contrast, the effective intra-layer coupling $\beta J_{\rm intra}$ exhibits much more complex thermal variations, which are for better illustration depicted in Fig. 2a) for several values of the AZFS parameter D/J. It can be directly proved from the definition (5) that $\beta J_{\rm intra}$ diverges as T^{-1} when reaching the zero temperature either according to the law $\beta J_{\rm intra} = 2J/(k_{\rm B}T)$ valid for $D/J > 0$, or according to the formula $\beta J_{\rm intra} = 2(D + J)/(k_{\rm B}T)$ valid for $D/J \in (-1, 0)$. Furthermore, the effective intra-layer coupling tends towards the constant value $\beta J_{\rm intra} = \ln 4$ when approaching the zero temperature for the special case $D/J = -1$, while it exponentially goes to zero by following the law $\beta J_{\rm intra} = 2\exp[(D + J)/(k_{\rm B}T)]$ in the region $D/J < -1$. Notice that all aforedescribed features can also be clearly seen in the dependences shown in Fig. 2a). This rather comprehensive analysis of the effective intra-layer coupling demonstrates that there does not exist (at least at the zero temperature) any effective intra-layer interaction between the spin-1/2 atoms if $D/J < -1$ and thus, the spin-1/2 atoms from the same layer should become completely independent of each other under this condition. This reasoning would have a simple physical explanation, since the relative strength of AZFS parameter $D/J = -1$ is just as strong as to make energy balance between the 'non-magnetic' ($S_{l,i} = 0$) and magnetic ($S_{l,i} = 1$) spin state of the decorating spins and accordingly, all vertex spins should be effectively separated by the 'non-magnetic' decorating spins $S_{l,i} = 0$ whenever $D/J < -1$.

Bearing all this in mind, one would intuitively expect that the layered Ising model on 3D decorated lattice must be disordered at any finite temperature when $D/J < -1$. Under this assumption, the only non-zero term at the zero temperature is the effective inter-layer interaction $J_{\text{inter}} = J'$ and the layered Ising model on 3D decorated lattice should therefore break into a set of the independent spin-1/2 Ising chains (running perpendicular to the layers) that do not possess a finite critical temperature. However, the mathematical structure of the critical condition (10) indicates a little bit more involved situation. The spin system is spontaneously ordered if the product on the left-hand-side of the critical condition (10) is greater than unity, while the spin system becomes disordered if it is less than unity. Thus, there exists a possibility that the product on the left-hand-side of the critical condition (10) might be greater than unity despite zero value of the effective intra-layer coupling, for instance, if a divergence of the effective inter-layer coupling βJ_{inter} overwhelms the asymptotic vanishing of the intra-layer coupling βJ_{intra}. One actually finds in the zero temperature limit ($T \to 0$ or equivalently $\beta \to \infty$) that

$$\lim_{\beta \to \infty} \left[\sinh\left(\frac{\beta J_{\text{intra}}}{2}\right) \sinh\left(\frac{\beta J_{\text{intra}}}{2} + \beta J_{\text{inter}}\right) \right] = \begin{cases} \infty & \text{if } \frac{D}{J} > -1 - \frac{J'}{J} \\ 0 & \text{if } \frac{D}{J} < -1 - \frac{J'}{J} \end{cases},$$

which means that the spontaneous order disappears only at $D/J = -1 - J'/J$ notwithstanding the simple intuitive expectations given above. Among other matters, this argument might serve in evidence of the outstanding spontaneous long-range ordering QFP that emerges in a range of the intermediate strong anisotropy parameters $D/J \in (-1 - J'/J, -1)$ despite the 'non-magnetic' nature of all decorating spins. For better illustration, Fig. 2b) shows in a graphical form several temperature dependences of the left-hand-side of the critical condition (10), which confirm correctness of the aforedescribed analysis for one particular value of the ratio $J'/J = 0.2$. It is noteworthy that this figure can also be regarded as a graphical solution of the critical condition (10) that determines a critical point of the layered Ising model on 3D decorated lattice as an intersection of both sides of the critical condition (10).

The finite-temperature phase diagram in a form of the dependence critical temperature vs. the anisotropy parameter D/J, which was obtained as a numerical solution of the critical condition (10), is shown in Fig. 3 for several values of the interaction ratio J'/J between the inter- and intra-layer interaction constants. It can be clearly seen from this figure that the critical temperature

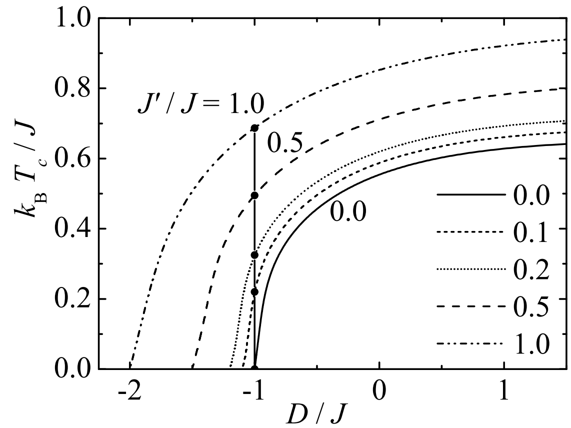

Fig. 3. The critical temperature as a function of the AZFS parameter D/J for several values of the ratio J'/J between the inter- and intra-layer interactions. The vertical line at $D/J = -1.0$ separates the displayed critical lines into two different regions that correspond to the FP ($D/J > -1.0$) and QFP ($D/J < -1.0$).

monotonically decreases with a decrease of the AZFS parameter D/J until it finally reaches the zero temperature at the boundary value $D/J = -1 - J'/J$, which is consistent with the one predicted by the ground-state analysis. The monotonic decrease of the critical temperature that occurs upon decrease of the AZFS term can simply be attributed to energetic favouring of thermal excitations to the 'non-magnetic' spin state $S_{l,i} = 0$. In addition, the vertical line at $D/J = -1$ must formally divide the depicted critical lines into two different region: the part on the right (i.e. for $D/J > -1$) is in fact a collection of the critical points that corresponds to the FP, while the part on the left (i.e. for $D/J < -1$) must correspond to the critical points of the QFP.

To provide an independent check of the aforementioned scenario, it might be quite useful to take a look at thermal dependences of the total and sublattice spontaneous magnetization. For this purpose, temperature variations of the total and sublattice magnetization are displayed in Fig. 4 for the particular value of the interaction ratio $J'/J = 0.2$ and several values of the anisotropy parameter D/J. Fig. 4a) shows thermal dependences of the total and sublattice magnetization, which are typical for $D/J \gtrsim 0$ and which lead to the most common Q-type temperature dependence of the total magnetization. On the other hand, the S-type temperature dependence of the total magnetization can be observed on assumption that the AZFS parameter is slightly greater than the boundary value $D/J = -1$ [see Fig. 4b) for $D/J = -0.9$]. The stair-like S-shaped dependence with a rapid initial decrease of the total magnetization obviously appears owing to preferred thermal excitations of the decorating spins to the 'non-magnetic' spin state $S_{l,i} = 0$. Namely, these thermal excitations are also reflected in the temperature dependence of the sublattice magnetization m_{B} and the 'non-magnetic' spin state $S_{l,i} = 0$ is close enough in energy to the spin state $S_{l,i} = 1$ to emerge in the ground state un-

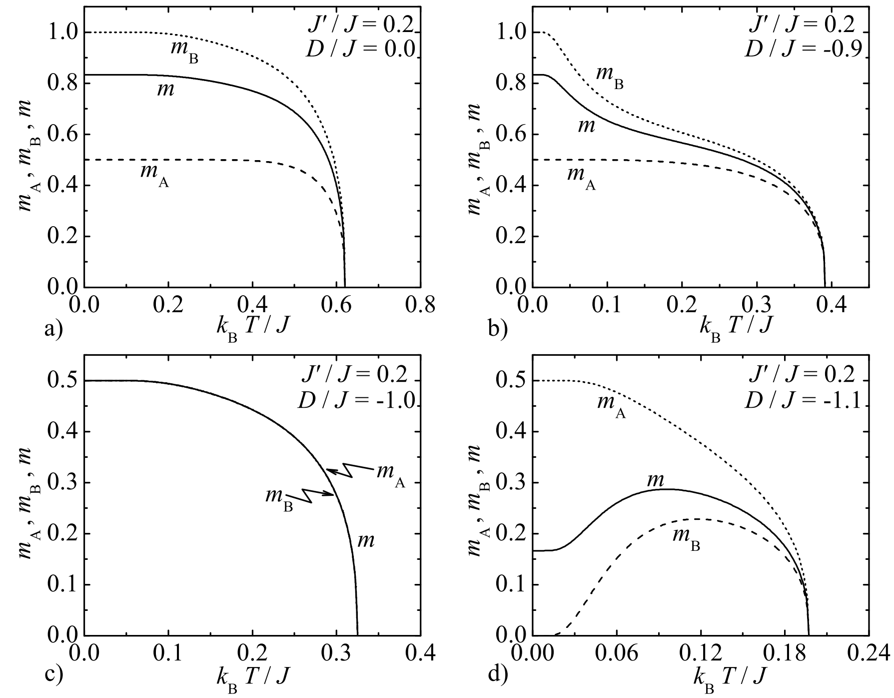

Fig. 4. Thermal dependences of the total magnetization m (solid lines) and the sublattice magnetization $m_{\rm A}$ (dashed lines), $m_{\rm B}$ (dotted lines) for the fixed value of the interaction ratio $J'/J = 0.2$ and several values of the AZFS parameter D/J.

der this condition. Interestingly, the standard thermal dependences of Q-type are recovered for the total and both sublattice magnetization by selecting the boundary value $D/J = -1$ (see Fig. 4c). It is worthwhile to remark, nevertheless, that the sublattice magnetization $m_{\rm B}$ pertinent to the decorating spins starts in this particular case from one half of its saturation value on behalf of the energetic equivalence between the spin states $S_{l,i} = 0$ and $S_{l,i} = 1$, which are populated with the same probability. Last but not least, the interesting L-type dependence of the total magnetization can be found for the anisotropy parameters $D/J < -1$ as depicted in Fig. 4d) for the particular case $D/J = -1.1$. As one can see from this figure, the sublattice magnetization $m_{\rm B}$ of the decorating spins starts from zero and this might be regarded as another convincing evidence of the existence QFP. Besides, the temperature-induced increase of the total magnetization evidently comes from the relevant thermal excitations of the decorating spins, which are clearly reflected in the thermal behaviour of the sublattice magnetization $m_{\rm B}$. In agreement with this suggestion, the observed temperature-induced increase of the magnetization is the more robust, the closer is the anisotropy parameter D/J to the boundary value $D/J = -1$, i.e. the closer in energy is the excited magnetic spin state $S_{l,i} = 1$ to the 'non-magnetic' spin state $S_{l,i} = 0$ emerging in the ground state.

Finally, we have also performed a rather detailed analysis of the critical behaviour by investigating critical exponents of the layered Ising model on 3D

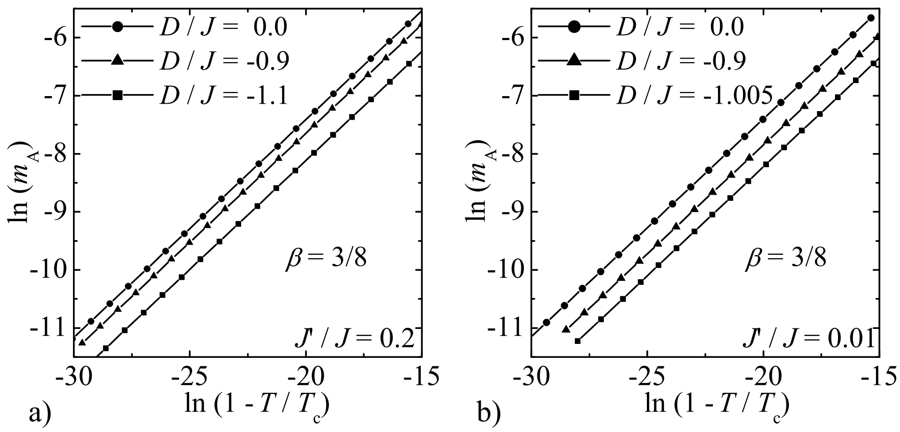

Fig. 5. The sublattice magnetization $m_{\rm A}$ versus the reduced temperature in a vicinity of critical points for $J'/J = 0.2$ (Fig. 5a) and 0.01 (Fig. 5b). The different symbols represent the magnetization vs. temperature data calculated for different anisotropy parameters D/J and the solid lines illustrate the best fit by linear curve with the slope (critical exponent) $\beta = 3/8$.

decorated lattice. It turned out that the investigated model system possesses the universal critical exponents, which are independent of the interaction parameters J, J', and D. This means that the same set of critical exponents characterizes the critical behaviour of the layered Ising model on 3D decorated lattice regardless of whether the standard FP or the unusual QFP is being the ground state. This fact becomes quite evident from Fig. 5, where the spontaneous magnetization $m_{\rm A}$ is plotted in a logarithmic scale against the reduced temperature for two different values of the interaction ratio J'/J and several values of the anisotropy parameter D/J. Apparently, the temperature variations of the spontaneous magnetization are in a vicinity of a critical point well fitted by the linear curves, which have the same critical exponent (slope) $\beta = 3/8$ irrespective of whether the FP ($D/J > -1$) or the QFP ($D/J < -1$) constitutes the ground state.

4 Conclusions

In the present work, the critical behaviour and magnetic properties of the layered Ising model of mixed spins on 3D decorated lattice are investigated by the use of generalized decoration-iteration transformation, which establishes a precise mapping relationship between the investigated model system and the corresponding spin-1/2 Ising model on the tetragonal lattice. It should be mentioned that recent conjectures on the exact solution of the spin-1/2 Ising model on the orthorhombic lattice [36], which contains as a special case the exact solution of the spin-1/2 Ising model on the tetragonal lattice, have enabled us to get accurately the critical and thermodynamic properties of the layered Ising model by maintaining essentially analytical form of the calculated quantities. In particular, the ground-state and finite temperature phase diagrams have been studied along with the possible temperature dependences of the total and sublattice magnetization.

The most interesting finding presented in this work surely represents a theoretical prediction of the striking spontaneous long-range ordering QFP, which appears in spite of the 'non-magnetic' nature of all decorating spins and the effectively 'quasi-1D' character of the spin system. It should be pointed out, however, that the analogous spontaneous long-range order of the effectively 'quasi-1D' spin system have already been exactly confirmed in the mixed-spin Ising model on a decorated square lattice with two different kinds of decorating spins on the horizontal and vertical bonds [49,50]. This noticeable and rather surprising coincidence can readily be understood from the mathematical structure of the critical condition (10), since the condition (10) of the spin-1/2 Ising model on the tetragonal lattice (10) formally coincides with the Onsager's critical condition [51] derived for the spin-1/2 Ising model on the anisotropic square (rectangular) lattice to which the mixed-spin Ising model on anisotropically decorated square lattice is effectively mapped [49,50].

Finally, it is worthwhile to remark that the presented exact solution can be rather straightforwardly extended to account for several additional interaction terms not included in the Hamiltonian (1) such as the biaxial zero-field splitting parameter acting on the decorating spins, the next-nearest-neighbour interaction between the vertex spins, the multispin interaction between the decorating spin and its two nearest-neighbour vertex spins and so on. In addition, the Zhang's putative exact solution for the spin-1/2 Ising model on the orthorhombic lattice [36] might be used to obtain accurate results for a whole set of the exactly solvable Ising models on 3D decorated lattices as well.

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