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

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Abstract

Phase transitions of the mixed spin-1/2 and spin-$S$ ($S \geq 1/2$) 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 yields for the layered Ising model of mixed spins plausible results either by adopting the conjectured solution for the spin-1/2 Ising model on the orthorhombic lattice [Z.-D. Zhang, Philos. Mag. 87 (2007) 5309-5419] or by performing extensive Monte Carlo simulations for the corresponding spin-1/2 Ising model on the tetragonal lattice. 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.

Key words: Ising model, decoration-iteration transformation, Monte Carlo simulations, phase transitions

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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 statistical 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 Ising models consists in a relative simple way 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 [3,4] 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 [5,6,7].

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 [8,9,10,11,12,13,14], multicompenation phenomenon [12,13,14,15], annealed disorder [16,17,18,19,20,21], as well as, the effect of non-zero external magnetic field [22,23,24]. 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. [25,26] 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 [27,28,29,30,31,32,33]. On the other hand, essentially exact results were recently reported by Oitmaa and Zheng [34] 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 \[35\]. 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 \[36\].

In the present work, the mixed spin-1/2 and spin-\(S\) Ising model on the layered 3D decorated lattice will be studied by applying the decoration-iteration transformation, which establishes a precise mapping relationship with the spin-1/2 Ising model on the tetragonal lattice. The reasonable results for the mixed-spin Ising model on the 3D decorated lattice can be consequently extracted from the corresponding results of much simpler spin-1/2 Ising model on the tetragonal lattice. Two alternative approaches are subsequently used for a theoretical analysis of the latter model: the first analytical approach is based on the Zhang’s conjectured solution for the spin-1/2 Ising model on the orthorhombic lattice \[37\], while the second numerical approach exploits Monte Carlo simulations. Even though there are serious doubts \[38,39,40\] about a rigour of the conjectured solution for the spin-1/2 Ising model on the 3D orthorhombic lattice \[37,41,42,43\], it is quite tempting to utilize it for a theoretical treatment of highly anisotropic spin systems because the Zhang’s results \[37\] correctly reproduce the Onsager’s exact solution for the spin-1/2 Ising model on the 2D rectangular lattice \[44\]. From this point of view, one should expect only small numerical error when treating highly anisotropic quasi-1D or quasi-2D spin systems even if the conjectured solution does not represent the true exact solution and moreover, the correctness of obtained results can easily be checked by the alternative numerical method based on the Monte Carlo simulations. The main advantage of the combination of the generalized decoration-iteration transformation with the Zhang’s conjectured solution is that it preserves the analytic form of the solution to be obtained for the layered Ising model of mixed spins. This advantage is naturally lost in the case of combining the decoration-iteration transformation with Monte Carlo simulations.

The outline of this paper is as follows. In Section 2 the detailed description of the layered mixed-spin Ising model is presented at first. Then, some details of the decoration-iteration mapping are clarified together with two alternative ways of how the magnetization and critical temperature can be calculated. The most interesting results are presented and detailed discussed in Section 3. Finally, some concluding remarks are mentioned in Section 4.
Fig. 1. Schematic representation of the mixed spin-1/2 and spin-S Ising model on the layered 3D decorated lattice and 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.

2 Ising model and its solution

Let us define the mixed spin-1/2 and spin-$S$ ($S \geq 1$) Ising model on the 3D layered 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 the horizontal bonds of the simple cubic lattice. Let us further denote the total number of layers by the symbol $L$, the total number of the spin-1/2 atoms within each layer as $N = L \times L$ and the total number of the spin-1/2 atoms as $N_T = L \times L \times L$. The model under investigation can be then defined through the Hamiltonian

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

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 $l$th layer at $j$th and $i$th lattice position, respectively, and periodic boundary conditions are imposed for simplicity. The parameter $J$ denotes the intra-layer interaction between the nearest-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 [45,46].

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

where \( \beta = 1/(k_B T) \), \( k_B \) 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]

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

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 \( J_{\text{intra}} \)

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

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

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 function

\[
Z(\beta, J, J', D) = A^{2NL} Z_{\text{tetragonal}}(\beta, J_{\text{intra}}, J_{\text{inter}} = J'). (6)
\]

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 \( J_{\text{intra}} \) 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 interlayer interaction $J_{\text{inter}}$ 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. [47,48,49,50], the sublattice magnetization $m_A$ 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

$$m_A(\beta, J, J', D) \equiv \langle \sigma_{l,i} \rangle_{\text{decorated}} = \langle \sigma_{l,i} \rangle_{\text{tetragonal}} \equiv m_0(\beta, J_{\text{intra}}, J_{\text{inter}}).$$

Above, the symbols $\langle \ldots \rangle_{\text{decorated}}$ and $\langle \ldots \rangle_{\text{tetragonal}}$ 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 $m_B$ of the spin-$S$ atoms can easily be calculated by combining the exact Callen-Suzuki spin identity [51,52] with the differential operator technique [53,54]. It is noteworthy that this kind of mathematical treatment essentially follows Kaneyoshi’s procedure [55] 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

$$m_B \equiv \langle S_{l,i} \rangle_{\text{decorated}} = 2m_A \sum_{n=-S}^{S} \frac{n \exp(\beta D n^2) \sinh(\beta J n)}{\sum_{n=-S}^{S} \exp(\beta D n^2) \cosh(\beta J n)}.$$

If both sublattice magnetization are known, the total magnetization of the mixed-spin Ising model on the 3D decorated lattice is given by the definition $m = (m_A + 2m_B)/3$.

It is quite obvious from Eqs. (7) and (8) that it is now sufficient to find the spontaneous magnetization of the corresponding spin-1/2 Ising model on the tetragonal lattice in order to complete our calculation of both sublattice magnetizations. For this purpose, we will utilize two alternative approaches: the first method adopts the conjectured solution for the spin-1/2 Ising model on the orthorhombic lattice [37], while the second method takes advantage of numerical Monte Carlo simulations. The former analytic procedure employs an explicit expression for the spontaneous magnetization of the spin-1/2 Ising model on the tetragonal lattice, which can be easily descended from the Zhang’s results for the spin-1/2 Ising model on the orthorhombic lattice [37].
\[ m_0 = \frac{1}{2} \left[ \frac{(1 - x^2 - x^2 y^4 + x^4 y^4)^2 - 16 x^4 y^4}{(1 - x^2)^2 (1 - x^2 y^4)^2} \right]^{3/8}, \]  

(9)

where \( x = \exp(-\beta J_{\text{intra}}/2) \) and \( y = \exp(-\beta J_{\text{inter}}/2) \). Within the framework of this analytic method, it is also easy to obtain the critical condition that thoroughly determines a critical point of the order-disorder phase transition of the layered Ising model on the 3D decorated lattice. Namely, both sub-lattice magnetization \( m_A \) and \( m_B \) 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 readily be found from the Zhang’s critical condition for the spin-1/2 Ising model on the orthorhombic lattice [37], which contains as a particular case the following critical condition for the spin-1/2 Ising model on the tetragonal lattice

\[ \sinh \left( \frac{\beta_c J_{\text{intra}}}{2} \right) \sinh \left( \frac{\beta_c J_{\text{intra}}}{2} + \beta_c J_{\text{inter}} \right) = 1, \]  

(10)

where \( \beta_c = 1/(k_B T_c) \) 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 \( J_{\text{intra}} \) satisfies the mapping relation (5) and the effective inter-layer interaction is equal to \( J_{\text{inter}} = J' \).

To avoid a danger of over-interpretation of the obtained results, the Monte Carlo simulations [56,57] were further used as the other alternative approach with the aim to provide an independent calculation of the spontaneous magnetization of the corresponding spin-1/2 Ising model on the tetragonal lattice defined via the effective interactions \( J_{\text{intra}} \) and \( J_{\text{inter}} \). The main advantage of a combination of the decoration-iteration transformation with the Monte Carlo method consists in a drastic reduction of the total Hilbert space, because the total number of available spin configurations reduces from \( [2(2S + 1)^2]^{N_T} \) to \( 2^{N_T} \) after performing the decoration-iteration transformation. Apparently, this drastic reduction of the total Hilbert space makes from the Monte Carlo simulations much more efficient tool for obtaining meaningful results. To be more specific, we have performed the Monte Carlo simulations for the spin-1/2 Ising model on the tetragonal lattice with the linear size \( L = 10, 20, 30, \) and 40. Note furthermore that periodic boundary conditions were imposed and all initial spin states were randomly assigned. The last spin configuration at any temperature was used as an input for maintained simulation at lower temperature. Spin configurations were generated by random passing through the tetragonal lattice and making single spin-flip attemps, which were accepted or rejected according to the standard Metropolis algorithm [58]. Finally, canon-
ical ensemble averages were calculated using $10^6$ Monte Carlo steps per site after discarding the initial $2 \times 10^5$ Monte Carlo steps per site.

The magnetization per site was calculated from the definition $m_0 = \langle |m_{MC}| \rangle \equiv (1/L^3) \langle |\sum_i \sigma_{l,i}| \rangle_L$, where the symbol $\langle \cdots \rangle_L$ denotes the ensemble average performed within the spin-1/2 Ising model on the tetragonal lattice with the linear size $L$. It is worthy to remind that the magnetization $m_0$ then directly equals to the sublattice magnetization $m_A$ relevant to the spin-1/2 atoms of the mixed-spin Ising model on 3D decorated lattice. The other sublattice magnetization $m_B$ of the spin-$S$ atoms can easily be enumerated from the relation [5]. For better accuracy, the critical temperature was determined with the help of fourth-order Binder cumulants $U_L = 1 - \langle m_{MC}^4 \rangle_L/[\langle m_{MC}^2 \rangle_L^2]$ [59,60], which intersect each other for different lattice sizes $L$ at a critical point according to the finite-size scaling theory [50].

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 the particular case with both ferromagnetic interaction constants $J > 0$ and $J' > 0$. It should be mentioned, however, that 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 the transformations $J \rightarrow -J$ and/or $J' \rightarrow -J'$, which merely cause 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.

First, let us take a closer look at finite-temperature phase diagrams, which are shown in Fig. 2 in the form of the critical temperature vs. the AZFS parameter dependences for several values of the decorating spins $S$ and the selected ratio $J'/J = 0.2$. In this figure, the solid lines depict analytical results obtained from the critical condition (10), while symbols connected by dotted lines show the corresponding numerical results acquired by the use of Monte Carlo simulations. It is quite obvious from Fig. 2 that the phase diagrams obtained from both independent theoretical approaches are in a good qualitative agreement, the numerical data for critical temperatures stemming from Monte Carlo simulations are in fact just slightly above the respective analyti-
Fig. 2. The critical temperature as a function of the AZFS parameter $D/J$ for several values of the decorating spins $S$ when the ratio between the inter- and intra-layer interactions is fixed to $J'/J = 0.2$. Solid lines depict the critical temperatures calculated from Eq. (10) of our analytical procedure, whereas symbols connected by dotted lines show the corresponding numerical results obtained by using Monte Carlo simulations.

Moreover, it can be also clearly seen from Fig. 2 that the overall critical behaviour basically depends merely on whether the decorating spins are half-odd-integer or integer ones. The critical temperature for the spin systems with half-odd-integer decorating spins (Fig. 2a) monotonically decreases upon decrease of the AZFS parameter until it asymptotically reaches the critical temperature of the special case with $S = 1/2$ that is of course independent of the AZFS parameter. This rather trivial finding can be straightforwardly attributed to a consecutive lowering of the spin state of the half-odd-integer decorating spins, which generally takes place at sufficiently strong negative values of the AZFS parameters $D/J = -1/(2n)$ on assumption that the relevant spin state changes from $S_{l,i} = n + 1/2$ to $S_{l,i} = n - 1/2$ ($n = 1, 2, 3, \ldots$).

Similarly, the critical temperature for the spin systems with integer decorating spins (Fig. 2b) monotonically decreases upon decrease of the AZFS parameter until it tends towards zero temperature at some boundary value of the AZFS parameter. The monotonous decrease of the critical temperature can be again explained in terms of a gradual decline of the spin state of integer decorating spins, which takes place at the following values of the AZFS parameter $D/J = -1/(2n - 1)$ provided that the spin state changes from $S_{l,i} = n$ to $S_{l,i} = n - 1$ ($n = 1, 2, 3, \ldots$). Contrary to our expectations, the critical temperatures of the spin systems with integer decorating spins do not vanish at the boundary value of the AZFS parameter, $D/J = -1$, below which all integer decorating spins tend towards their ‘non-magnetic’ spin state $S_{l,i} = 0$. This is the most remarkable finding of our study and we will henceforth explore this striking critical behaviour, which represents a general feature of the spin systems with integer decorating spins, on the simplest model with the integer decorating spins $S = 1$. 

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Let us consider first possible spin arrangements to emerge in the ground state of this particular model system. It turns out that three different phases may appear in total at zero temperature in dependence on a relative strength of the intra-layer interaction $J$, the inter-layer interaction $J'$, and the AZFS 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 $D/J > -1$. Note that this finding is consistent with the relevant results of our analytical approach as well as the numerical Monte Carlo simulations. On the other hand, it directly follows from the critical condition (10) that 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 $(S_{l,i}; \sigma_{l,i}) = (0; 1/2)$. It should be stressed that the qualitatively same behaviour is also predicted by Monte Carlo simulations even although it becomes rather hard to estimate accurately the lower boundary of QFP within this numerical technique (see for details the subsequent part). The absence of any spontaneous long-range order can finally be detected in the disordered phase (DP), which becomes the lowest-energy state on assumption that $D/J < -1 - J'/J$ when the critical condition (10) is taken into account. 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 resulting from our 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 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 $\beta J_{\text{intra}}$ and $\beta J_{\text{inter}}$ of the corresponding spin-1/2 Ising model on the tetragonal lattice, which were used both in our analytical approach as well as Monte Carlo simulations. The effective inter-layer coupling $\beta J_{\text{inter}} = J'/(k_B T)$ 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 $\beta J_{\text{intra}}$ exhibits much more complex thermal variations, which are for better illustration depicted in Fig. 3a) for several values of the AZFS parameter $D/J$. It can be directly proved from the definition (3) that $\beta J_{\text{intra}}$ diverges as $T^{-1}$ when reaching the zero temperature either according to the law $\beta J_{\text{intra}} = 2J/(k_B T)$ valid for
**Fig. 3.** Typical temperature dependences of the effective intra-layer coupling $\beta J_{\text{intra}}$ are shown in Fig. 3a) for several values of the AZFS parameter $D/J$. Note that $\beta J_{\text{intra}}$ is given by the mapping relation (5) and it does not depend on a strength of the inter-layer interaction $J'$. Fig. 3b) 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 for several values of the AZFS parameter $D/J$ and the ratio $J'/J = 0.2$. The points of intersection between broken and solid lines (full circles) determine critical points.

$D/J > 0$, or according to the formula $\beta J_{\text{intra}} = 2(D + J)/(k_B T)$ valid for $D/J \in (-1, 0)$. Furthermore, the effective intra-layer coupling tends towards the constant value $\beta J_{\text{intra}} = \ln 4$ when approaching zero temperature for the special case $D/J = -1$, while it exponentially goes to zero by following the law $\beta J_{\text{intra}} = 2 \exp[(D + J)/(k_B T)]$ in the region $D/J < -1$. Notice that all aforedescribed features can also be clearly seen in the dependences shown in Fig. 3b). This comprehensive analysis of the effective intra-layer coupling demonstrates that there does not exist (at least at 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 struc-
ture of the critical condition (10) as well as the numerical results from Monte Carlo simulations indicate a more involved situation. Our analytical approach implies that the spin system is spontaneously ordered (disordered) if the product on the left-hand-side of the critical condition (10) is greater (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 the zero value of the effective intra-layer coupling, for instance, if a divergence of the effective inter-layer coupling $\beta J_{\text{inter}}$ overwhelms the asymptotic vanishing of the intra-layer coupling $\beta J_{\text{intra}}$. 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. 3b) shows in a graphical form several temperature dependences of the left-hand-side of the critical condition (10) for one particular value of the ratio $J'/J = 0.2$, which confirm a correctness of the aforedescribed analysis. 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 Eq. (10). Finally, it is worth noticing that the above mentioned analysis is also consistent with the numerical results of Monte Carlo simulations, which predict the spontaneous order for intermediate values of the AZFS parameter $D/J \lesssim -1$ as well.

For comparison, we depict in Fig. 4 the critical temperature as a function of the AZFS parameter for the particular spin case $S = 1$ and two different values of the interaction ratio $J'/J = 0.0$ and 0.2. The critical temperatures, which are displayed in Fig. 4 as solid and dashed lines, were obtained by numerically solving the critical condition (10). The symbols connected by dotted lines depict the relevant numerical data obtained by using Monte Carlo simulations. It is worthwhile to remark that the critical line displayed in Fig. 4 for the special case $J'/J = 0$ is fully consistent with the formerly published exact results [12,15]. In this particular case, the critical line actually ends up at the expected ground-state boundary $D/J = -1$ at which the spin state $S_{l,i} = 1$ changes to the 'non-magnetic' one $S_{l,i} = 0$ and there does not appear a striking spontaneous order inherent to QFP. This is a direct consequence of the fact that the critical condition (10) extracted from the Zhang’s solution for
Fig. 4. The critical temperature as a function of the AZFS parameter $D/J$ for the particular spin case $S = 1$ and two different values of the ratio $J'/J = 0.0$ and 0.2 between the inter- and intra-layer interactions. The solid and dashed lines without any symbol show the critical lines obtained from Eq. (10). The symbols connected by dotted lines display the relevant critical points acquired from Monte Carlo simulations.

the spin-1/2 Ising model on the orthorhombic lattice essentially reduces to the famous Onsager’s solution for the spin-1/2 Ising model on the square lattice. It should be pointed out, moreover, that the relevant numerical data from Monte Carlo simulations are lying on this critical line, which confirms accuracy of our Monte Carlo simulations. The critical temperature monotonically decreases with a decrease of the AZFS parameter also for any non-zero inter-layer interaction $J'/J \neq 0$ until it tends to zero at some stronger (more negative) values of the AZFS parameter (see the curve for the particular case $J'/J = 0.2$). This surprising finding is evident both from our analytical results as well as Monte Carlo simulations. However, the decorating spins reside the spin state $S_{l,i} = 1$ just if $D/J > -1$, while they reside the ‘non-magnetic’ spin state $S_{l,i} = 0$ whenever $D/J < -1$. From this perspective, the boundary value of the AZFS parameter $D/J = -1$ divides the critical line into two different region: the part where $D/J > -1$ corresponds to the critical points of the FP, while the part where $D/J < -1$ corresponds to the critical points of the QFP. It should be also mentioned that the lower boundary allocating a presence of the spontaneously ordered QFP is $D/J = -1 - J'/J$ according to the critical condition, while it becomes rather hard to locate precisely the lower boundary with the help of Monte Carlo simulations. Namely, the more and more extensive Monte Carlo simulations are needed at sufficiently low temperatures in order to overcome finite-size effects that become very important in the parameter space $D/J < -1$, because the relevant spin system effectively splits into a set of weakly interacting spin-1/2 Ising chains running perpendicular to the layers.

To provide an independent check of a presence of spontaneously ordered QFP, it might be quite useful to take a look at thermal dependences of the total
and sublattice spontaneous magnetizations. For this purpose, some temperature variations of the total and sublattice magnetizations are displayed in Fig. 5 for the particular value of the interaction ratio $J'/J = 0.2$ and several values of the AZFS parameter $D/J$. It is noteworthy that the results obtained from our analytical procedure are in a good qualitative accordance with the numerical estimates of Monte Carlo simulations. However, there appears just a small deviation between the relevant results at relatively high temperatures close to a critical point, because our analytical procedure slightly underestimates the critical temperature in comparison with the Monte Carlo predictions. Fig. 5a) shows thermal dependences of the total and sublattice magnetizations, 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. 5b) 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 under this condition. Interestingly, the standard thermal dependences of Q-type are recovered for the total and both sublattice magnetizations by selecting the boundary value $D/J = -1$ (see Fig. 5c). It is worthwhile to remark, nevertheless, that the sublattice magnetization $m_B$ 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. As a result, both sublattice magnetization exhibit the qualitatively same dependences that cannot be distinguished within the displayed scale. Last but not least, the interesting L-type dependence of the total magnetization can be found for the AZFS parameters $D/J < -1$ as depicted in Fig. 5d) for the particular case $D/J = -1.05$. As one can see from this figure, the sublattice magnetization $m_B$ 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 $m_B$. In agreement with this suggestion, the observed temperature-induced increase of the magnetization is the more robust, the closer is the AZFS parameter 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 at $T = 0$.

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. This exact mapping method was subsequently combined either with the conjectured solution for the spin-1/2 Ising model on the orthorhombic lattice [37] or numerical Monte Carlo simulations with the aim to obtain the meaningful results for the mixed-spin Ising model on the layered 3D decorated lattice. The main advantage of the former procedure is that it preserves essentially analytical form of the results obtained for critical and thermodynamic properties of the layered mixed-spin Ising model, while the main advantage of the latter procedure rest in a drastic reduction of the total Hilbert space that makes Monte Carlo simulations very efficient. In the spirit of both these techniques, the ground-state and finite temperature phase diagrams have been studied along with possible temperature dependences of the total and sublattice magnetizations.
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 [61,62]. This noticeable and rather surprising coincidence can readily be understood from the mathematical structure of the critical condition (10). Indeed, the proposed critical condition (10) for the spin-1/2 Ising model on the tetragonal lattice formally coincides with the Onsager’s critical condition [44] 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 [61,62].

Finally, it is worthwhile to remark that the presented solution can be rather straightforwardly extended to account for several additional interaction terms not included in the Hamiltonian (11) 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.

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