Magnetic properties of exactly solvable doubly decorated Ising-Heisenberg planar models

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Applying the decoration-iteration procedure, we introduce a class of exactly solvable doubly decorated planar models consisting both of the Ising- and Heisenberg-type atoms. Exact solutions for the ground state, phase diagrams, and basic physical quantities are derived and discussed. The detailed analysis of the relevant quantities suggests the existence of an interesting quantum antiferromagnetic phase in the system.

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I. INTRODUCTION

The quantum Heisenberg model (QHM) (Ref. 1) and its simplified Ising version[2] remain one of the most actively studied subjects in statistical mechanics. In particular, the low-dimensional antiferromagnetic QHM has recently attracted a lot of attention since it represents a very useful model for the investigation of interesting quantum phenomena. Among the most fascinating problems that are of current interest in this field, one should mention the investigation of Haldane gaps in the one-dimensional (1D) antiferromagnetic QHM with integer spins,[3] quantum phase transitions,[4] spin-Peierls instabilities,[5] dimerization and other related phenomena,[6] quantum entanglement,[7] magnetization plateaus,[8] and so on. In addition to the above mentioned works, a number of the studies has been devoted to the investigation of the role of magnetic ordering in high-T_c superconducting cuprates consisting of two-dimensional Cu-O networks.[9] In fact, the magnetic properties of these materials can be well described by means of a spin-1/2 antiferromagnetic 2D QHM.

Despite of extensive studies, the QHM has been exactly solved in one dimension only[10]; thus for higher dimensions only more or less accurate approximate methods are available.[11] In general, the main difficulties of a rigorous treatment of the QHM are closely associated with the noncommutability of the spin operators involving the Hamiltonian of the system. This principal mathematical intractability of the QHM has motivated us to introduce a class of interesting exactly solvable models, consisting both of the Ising- and Heisenberg-type atoms. For this purpose, we utilize the well known decoration-iteration procedure originally introduced by Syozi[12] and later remarkably generalized by Fisher.[13] In the spirit of the Syozi's and Fishers's papers, in this work we use the decoration procedure to put a couple of Heisenberg atoms on each bond of the regular Ising lattice. In this way we obtain a doubly decorated model consisting of two interpenetrating sublattices occupied by Ising- and Heisenberg-type atoms, respectively, and such a model can be of interest both theoretically and experimentally. Theoretically, the most outstanding feature of this model is the fact that it enables to investigate, by an exact calculation, how the quantum Heisenberg atoms modify the magnetic properties of the pure Ising systems. On the other hand, from the experimental point of view, the model can be inspiring in the preparation of new magnetic materials with similar topological structure as the system under investigation. Actually, some of recently synthesized compounds represent a progressive step in this direction.[14]

The outline of the present paper is as follows. In Sec. II, the main points of the mathematical formulation of the decoration-iteration procedure for Ising-Heisenberg models are explained and the exact equation for the phase diagrams and basic physical quantities are derived. The most interesting numerical results are presented and discussed in detail in Sec. III, and, finally, some concluding remarks are given in Sec. IV.

II. FORMULATION

In this work we will study the spin-1/2 Ising-Heisenberg model on planar doubly decorated lattices. In order to illustrate a typical topological structure of the considered system, in Fig. 1 we depict a part of the doubly decorated square lattice. In this figure the black circles denote the spin-1/2 Ising atoms that occupy the sites of the original square lattice and the gray ones represent the spin-1/2 Heisenberg atoms residing on the bonds of the original lattice.

Consequently, the Hamiltonian of the Ising-Heisenberg model can be written in the form

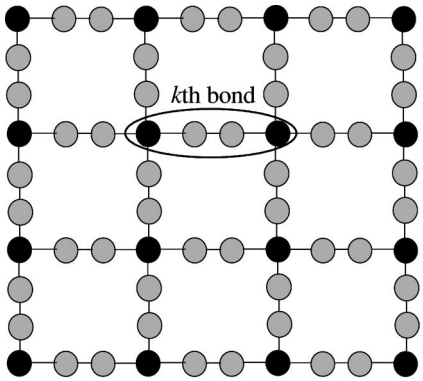

FIG. 1. The fragment of the doubly decorated square lattice. The black (gray) circles denote the positions of the Ising (Heisenberg) atoms, respectively. The ellipse demarcates a typical bond described by the Hamiltonian $\hat{\mathcal{H}}_k$ [see Eq. (2)].

$$\hat{\mathcal{H}}_d = -\frac{1}{2}\sum_{i,j} J_{ij}[\Delta(\hat{S}_i^x\hat{S}_j^x+\hat{S}_i^y\hat{S}_j^y)+\hat{S}_i^z\hat{S}_j^z] - \frac{1}{2}\sum_{k,\not\ell} J_{k\not\ell}^{(1)}\hat{\mu}_k^z\hat{S}_{\not\ell}^z, \tag{1}$$

where both summations in the first term are carried out over all Heisenberg atoms. On the other hand, in the second term the first summation runs over all Ising atoms and the second one over all Heisenberg atoms. As usual, in this work we restrict all possible interactions to the nearest-neighboring atoms only. For this purpose we set $J_{ij}=J$ if the site i is the nearest neighbor of the site j. Otherwise we assume that $J_{ij}=0$. Similarly, for nearest-neighboring sites k and $\not\ell$ we put $J_{k\not\ell}^{(1)}=J_1$ and $J_{k\not\ell}^{(1)}=0$ in all other cases. The factor 1/2 in both terms of Eq. (1) has been included to avoid double-counting of the relevant terms. Finally, $\hat{S}_i^\alpha$ and $\hat{\mu}_l^z$ represent the well-known components of spin-1/2 operators, and Δ describes the spatial anisotropy in the Heisenberg exchange interaction. In fact, this parameter allows one to control the behavior of the system between the Ising regime for $\Delta<1$ (easy-axis-like anisotropy) and the XY regime for $\Delta>1$ (easy-plane anisotropy). In view of further manipulations, it is useful to rewrite the total Hamiltonian of the system as a sum of the bond Hamiltonians, i.e., $\hat{\mathcal{H}}_d=\Sigma_k\hat{\mathcal{H}}_k$, where the summation is carried out over all the pairs of Heisenberg atoms. The bond Hamiltonian $\hat{\mathcal{H}}_k$ involves all the interaction terms associated with the kth pair of Heisenberg atoms (see Fig. 1), and is given by

$$\begin{aligned}\hat{\mathcal{H}}_k = &-J[\Delta(\hat{S}_{k1}^x\hat{S}_{k2}^x+\hat{S}_{k1}^y\hat{S}_{k2}^y)+\hat{S}_{k1}^z\hat{S}_{k2}^z]\\ &-J_1(\hat{S}_{k1}^z\hat{\mu}_{k1}^z+\hat{S}_{k2}^z\hat{\mu}_{k2}^z).\end{aligned} \tag{2}$$

The most important point of our treatment is the calculation of the partition function for the system under investigation. Taking into account the standard commutation relation for the bond Hamiltonians (i.e., $[\hat{\mathcal{H}}_i,\hat{\mathcal{H}}_k]=0,\ i\neq k$), we can express the partition function $\mathcal{Z}_d$ of decorated system in the form

$$\begin{aligned}\mathcal{Z}_d &= \mathrm{Tr}\exp(-\beta\hat{\mathcal{H}}_d)=\mathrm{Tr}\exp\left(-\beta\sum_{k=1}^{Nq/2}\hat{\mathcal{H}}_k\right)\\ &= \mathrm{Tr}_{\{\mu\}}\prod_{k=1}^{Nq/2}\mathrm{Tr}_{S_{k1}}\mathrm{Tr}_{S_{k2}}\exp(-\beta\hat{\mathcal{H}}_k),\quad \beta=1/k_BT,\end{aligned} \tag{3}$$

where k_B is the Boltzmann constant and T the absolute temperature. N represents the total number of Ising atoms and q is the coordination number of the original (undecorated) lattice. The symbol $\mathrm{Tr}_{\{\mu\}}$ means a trace over all degrees of freedom of Ising spins and finally, $\mathrm{Tr}_{S_{k1}}\mathrm{Tr}_{S_{k2}}$ denotes a trace over a couple of Heisenberg spins residing on the kth bond. To proceed further, it is useful to introduce the following extended decoration-iteration transformation:[12,13]

$$\begin{aligned}&\mathrm{Tr}_{S_{k1}}\mathrm{Tr}_{S_{k2}}\exp(-\beta\hat{\mathcal{H}}_k)\\ &\quad= 2\exp(\beta J/4)\Big\{\cosh[\beta J_1(\mu_{k1}^z+\mu_{k2}^z)/2]\\ &\qquad+\exp(-\beta J/2)\cosh\left[\frac{\beta}{2}\sqrt{J_1^2(\mu_{k1}^z-\mu_{k2}^z)^2+J^2\Delta^2}\right]\Big\}\\ &\quad= A\exp(\beta R\mu_{k1}^z\mu_{k2}^z).\end{aligned} \tag{4}$$

The unknown transformation parameters A and R can be easily obtained following the standard procedures (see Ref. 12 and references therein), namely,

$$A=2\exp(\beta J/4)(V_1V_2)^{1/2},\quad \beta R=2\ln\left(\frac{V_1}{V_2}\right), \tag{5}$$

where we have introduced the functions V_1 and V_2 as follows:

$$\begin{aligned}V_1 &= \cosh(\beta J_1/2)+\exp(-\beta J/2)\cosh(\beta J\Delta/2),\\ V_2 &= 1+\exp(-\beta J/2)\cosh\left(\frac{\beta}{2}\sqrt{J_1^2+J^2\Delta^2}\right).\end{aligned} \tag{6}$$

Now, after substituting Eq. (4) into Eq. (3) one obtains the equation

$$\mathcal{Z}_d=A^{Nq/2}\mathcal{Z}_0, \tag{7}$$

which relates the partition function of the doubly decorated Ising-Heisenberg model ($\mathcal{Z}_d$) to that of the original undecorated spin-1/2 Ising model ($\mathcal{Z}_0$.) From this simple relation, we can directly calculate some physical quantities (for example, the free and internal energies or specific heat) on the basis of well-known thermodynamic relations. However, to understand the behavior of the system, we have to analyze also some other quantities (for instance the magnetization and pair-correlation functions) that cannot be obtained from the partition function in a straightforward manner. Fortunately, we can avoid this complication by exploiting the exact identities

$$\langle f_1(\hat{\mu}_i^z,\hat{\mu}_j^z,\ldots,\hat{\mu}_k^z)\rangle_d=\langle f_1(\hat{\mu}_i^z,\hat{\mu}_j^z,\ldots,\hat{\mu}_k^z)\rangle_0, \tag{8}$$

$$\begin{aligned}&\langle f_2(\hat{S}_{k1}^\alpha,\hat{S}_{k2}^\gamma,\hat{\mu}_{k1}^z,\hat{\mu}_{k2}^z)\rangle_d\\ &\quad=\left\langle\frac{\mathrm{Tr}_{S_{k1}}\mathrm{Tr}_{S_{k2}}f_2(\hat{S}_{k1}^\alpha,\hat{S}_{k2}^\gamma,\hat{\mu}_{k1}^z,\hat{\mu}_{k2}^z)\exp(-\beta\hat{\mathcal{H}}_k)}{\mathrm{Tr}_{S_{k1}}\mathrm{Tr}_{S_{k2}}\exp(-\beta\hat{\mathcal{H}}_k)}\right\rangle_d,\end{aligned} \tag{9}$$

from which the relevant quantities can be calculated. In the above equations, f_1 represents a function depending only on the Ising spin variables, and f_2 denotes a function which depends on the spin variables located on the kth bond only. The superscripts α and γ denote x,y or z components of the spin operators and the symbols $\langle\cdots\rangle_d$ and $\langle\cdots\rangle_0$ mean the standard ensemble average related to the decorated and origi-

nal lattice, respectively. Now, applying one of the standard methods,[15] we simply derive equations for the sublattice magnetization,

$$m_A^z \equiv \frac{1}{2}(\langle \hat{\mu}_{k1}^z + \hat{\mu}_{k2}^z \rangle_d) = \frac{1}{2}(\langle \hat{\mu}_{k1}^z + \hat{\mu}_{k2}^z \rangle_0) = m_0, \quad (10)$$

$$m_B^z \equiv \frac{1}{2}\langle \hat{S}_{k1}^z + \hat{S}_{k2}^z \rangle_d = 8(\langle \hat{\mu}_{k1}^z \rangle_d + \langle \hat{\mu}_{k2}^z \rangle_d) K_0, \quad (11)$$

$$m_B^x \equiv \frac{1}{2}\langle \hat{S}_{k1}^x + \hat{S}_{k2}^x \rangle_d = 0, \quad (12)$$

$$m_B^y \equiv \frac{1}{2}\langle \hat{S}_{k1}^y + \hat{S}_{k2}^y \rangle_d = 0, \quad (13)$$

where m_0 is the magnetization per one site of the original lattice and the coefficient K_0 is given in the Appendix. Similarly, the various pair correlations can be expressed with the help of Eqs. (8) and (9) in the simple forms

$$q_{ii}^{zz} \equiv \langle \hat{\mu}_{k1}^z \hat{\mu}_{k2}^z \rangle_d = \langle \hat{\mu}_{k1}^z \hat{\mu}_{k2}^z \rangle_0 \equiv \varepsilon, \quad (14)$$

$$q_{hh}^{xx} \equiv \langle \hat{S}_{k1}^x \hat{S}_{k2}^x \rangle_d = K_1 + K_2 + 4q_{ii}^{zz}(K_1 - K_2), \quad (15)$$

$$q_{hh}^{yy} \equiv \langle \hat{S}_{k1}^y \hat{S}_{k2}^y \rangle_d = q_{hh}^{xx}, \quad (16)$$

$$q_{hh}^{zz} \equiv \langle \hat{S}_{k1}^z \hat{S}_{k2}^z \rangle_d = K_3 + K_4 + 4q_{ii}^{zz}(K_3 - K_4), \quad (17)$$

$$q_{ih}^{zz} \equiv \frac{1}{2}\langle \hat{S}_{k1}^z \hat{\mu}_{k1}^z + \hat{S}_{k2}^z \hat{\mu}_{k2}^z \rangle = K_0 + K_5 + 4q_{ii}^{zz}(K_0 - K_5). \quad (18)$$

Here $\varepsilon \equiv \langle \hat{\mu}_{k1}^z \hat{\mu}_{k2}^z \rangle_0$ denotes the nearest neighbor correlation of the original lattice that is well known and the coefficients $K_0 - K_5$ are listed in the Appendix. Finally, the internal energy and specific heat of the system can be also easily calculated from the relations

$$U_d = -\frac{Nq}{2}[J\Delta(q_{hh}^{xx} + q_{hh}^{yy}) + Jq_{hh}^{zz} + 2J_1 q_{ih}^{zz}], \quad (19)$$

$$C_d = \partial U_d / \partial T. \quad (20)$$

III. NUMERICAL RESULTS AND DISCUSSION

In this section we will show the most interesting numerical results of the system under investigation. For the sake of simplicity, we restrict our attention to case of the doubly decorated square lattice (see Fig. 1) in which all characteristic properties can be illustrated.

Before discussing the results, it is worth noticing that the phase diagrams for the ferromagnetic ($J>0, J_1>0$) and ferrimagnetic ($J>0, J_1<0$) case will be the same, since the relevant equation for the critical temperature is invariant under the transformation $J_1 \leftrightarrow -J_1$. On the other hand, the antiferromagnetic system ($J<0$ and arbitrary J_1) exhibits many different features and will be discussed in a separate work.

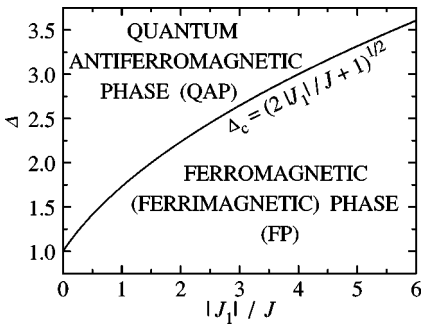

FIG. 2. Ground-state phase diagram of the doubly decorated Ising-Heisenberg model. The full lines represents the line of first-order phase transitions that separates the ferromagnetic or ferrimagnetic phase (FP) from the quantum antiferromagnetic phase (QAP).

In order to find possible ground state phases and to investigate their properties, we have to analyze the internal energy, magnetization and correlation functions at $T=0$. Depending on whether the anisotropy parameter Δ is less than, equal to, or greater than the boundary value $\Delta_c = \sqrt{2|J_1|/J+1}$ one finds three different regions.

(i) For $\Delta < \Delta_c$,

$$U_d = -\frac{Nq}{8}(2|J_1| + J),$$

$$q_{ii}^{zz} = q_{hh}^{zz} = 0.25, \quad q_{ih}^{zz} = \pm 0.25, \quad q_{hh}^{xx} = q_{hh}^{yy} = 0.0. \quad (21)$$

(ii) For $\Delta > \Delta_c$

$$U_d = -\frac{Nq}{8}[-J + 2\sqrt{J_1^2 + (J\Delta)^2}],$$

$$q_{ii}^{zz} = q_{hh}^{zz} = -0.25, \quad q_{ih}^{zz} = \pm \frac{J_1}{4\sqrt{J_1^2 + (J\Delta)^2}},$$

$$q_{hh}^{xx} = q_{hh}^{yy} = \frac{J\Delta}{4\sqrt{J_1^2 + (J\Delta)^2}}. \quad (22)$$

(iii) for $\Delta = \Delta_c$,

$$U_d = -\frac{Nq}{8}(2|J_1| + J),$$

$$q_{ii}^{zz} = q_{hh}^{zz} = 0.0, \quad q_{ih}^{zz} = \pm \frac{2|J_1| + J}{8(|J_1| + J)},$$

$$q_{hh}^{xx} = q_{hh}^{yy} = \frac{\sqrt{J(|J_1| + J)}}{8(|J_1| + J)}. \quad (23)$$

The plus or minus sign one applies for the ferromagnetic or ferrimagnetic case, respectively. From these relations, we have obtained the ground-state phase diagram in the $|J_1| - \Delta$ space which is depicted in Fig. 2. Taking into account Eqs. (21)–(23), one easily identifies the standard ferromagnetic (ferrimagnetic) phase (FP) for $\Delta < \Delta_c$. However, for $\Delta > \Delta_c$ an unexpected quantum phase occurs in the system.

This phase [to be referred to as a quantum antiferromagnetic phase (QAP)] requires more detailed description since it differs from standard phases in the pure Ising or Heisenberg models and, as far as we know, such a phase has not been described in the literature before. In fact, from the relevant equations we find that in the QAP the Ising spins (that are the nearest neighbors on the original lattice) are aligned antiparallel with respect to each other. Consequently, we have the classical Néel long-range ordering on the Ising sublattice with $m_A=0.0$ and $q_{ii}^{zz}=-0.25$. On the other hand, the nearest-neighboring Heisenberg spins create dimers, thus we also have $m_B=0.0$ and $q_{hh}^{zz}=-0.25$. However, the alignment of these dimers with respect to their nearest-neighboring Ising spins is random; hence the relevant correlation function q_{ih}^{zz} does not reach its saturated value (± 0.25). Moreover, one easily observes that the degree of randomness increases with the increasing in anisotropy Δ. This behavior apparently appears due to the competition between strong easy-plane anisotropy (Δ) that supports short-range ordering and the exchange interactions (J, J_1) ''preferring'' the long-range ordering along the easy axis. It is also clear from the aforementioned arguments that despite of some disorder introduced by random orientation of the dimers, the QAP will exhibit the long-range Néel ordering captured to the Ising spins. Thus one can expect the appearance of the second-order phase transition in the system at finite temperatures, even for very strong values of the anisotropy parameter Δ. Nevertheless, the QAP also differs from the standard Néel phase (both the classical and quantum one) due to the ferromagnetic in-plane short-range order of the Heisenberg spins. Another unusual feature of the QAP is the perfect antiparallel alignment of the Ising spins (that are not directly coupled via exchange), despite some disorder present between the nearest-neighboring Ising and Heisenberg atoms. Furthermore, we would like to emphasize that the existence of the QAP by itself is very surprising, since we have the system with the ferromagnetic exchange interactions J and J_1 only.

Finally, one should notice that the FP and QAP are separated by the first-order phase transition line that is given by the condition $\Delta=\Delta_c=\sqrt{2|J_1|/J+1}$. At an arbitrary point of this line there coexist two of the above mentioned phases (FP, QAP) together with a disordered phase (DP) in which we have $m_A^z=m_B^z=q_{ii}^{zz}=q_{hh}^{zz}=0.0$ and the nonvanishing short-range ordering both in the xy plane and along the easy axis $(q_{hh}^{xx}=q_{hh}^{yy}\neq 0,\ q_{ih}^{zz}\neq 0)$. The coexistence of these three phases follows from the fact that the relevant ground-state energies take the same value [in fact, $\lim_{\Delta\to\Delta_c^-}U_d(\mathrm{FP})=\lim_{\Delta\to\Delta_c^+}U_d(\mathrm{QAP})=U_d(\mathrm{DP})_{\Delta=\Delta_c}$].

Next, in order to demonstrate the overall dependences of the correlation functions on the anisotropy parameter Δ, we have depicted in Fig. 3 the relevant pair correlations for the case $J_1/J=1.0$. In agreement with the arguments given above, we find the FP for $\Delta<\sqrt{3}$ and the QAP for $\Delta>\sqrt{3}$. Moreover, Fig. 3 indicates that for $\Delta>\sqrt{3}$, the correlations q_{ih}^{zz} decrease with the increasing Δ and vanish in the limit of $\Delta\to\infty$. On the other hand, the correlation q_{hh}^{xx} increases with the parameter Δ and approaches its saturation value for Δ $\to\infty$. Contrary to this behavior, the correlations q_{ii}^{zz} and q_{hh}^{zz} take saturation values independently of Δ, excepting the special point $\Delta=\Delta_c$ where they jump to zero. Thus, the antiparallel orientation of the relevant Ising and Heisenberg spin pairs is not affected at all even by the very strong anisotropy. Finally, to complete the ground-state analysis, in Fig. 4 we show the internal energy of different phases as a function of the anisotropy parameter Δ for $|J_1|/J=1.0$. In this figure, the full and dashed lines represent the stable and unstable parts of the relevant energies, respectively. The black point is the energy of the DP. This dependence apparently supports our previous statements and clearly illustrates the occurrence of the first-order phase transition at $\Delta=\Delta_c=\sqrt{3}$.

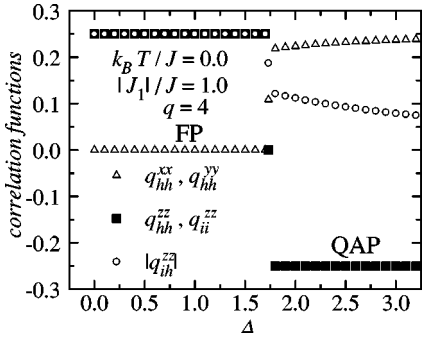

FIG. 3. Dependences of the pair-correlation functions at the front state on the anisotropy parameter Δ for the doubly decorated square lattice $(q=4)$ and $|J_1|/J=1.0$.

Now let us proceed to study the finite-temperature phase diagrams for $q=4$ that can be easily obtained by putting $\beta_c R=\pm 2\ln(1+\sqrt{2})$ into Eq. (5). Solving the relevant equation numerically for some characteristic values of J_1, we have obtained the phase boundaries in the $\Delta-T_c$ plane that are plotted in Fig. 5. As one can see, the critical temperature decreases gradually from its Ising value at $\Delta=0$ and vanishes for $\Delta=\Delta_c=\sqrt{2|J_1|/J+1}$. On the other hand, for $\Delta>\Delta_c$ the transition temperature at first rapidly increases, then passes through a local maximum value and finally tends to zero for $\Delta\to\infty$. It is clear that for $\Delta<\Delta_c$ the phase boundary separates the FP and DP, and similarly for $\Delta>\Delta_c$ separates QAP and DP. As one can expect, the relevant thermal phase transition is of the second order and belongs to the same

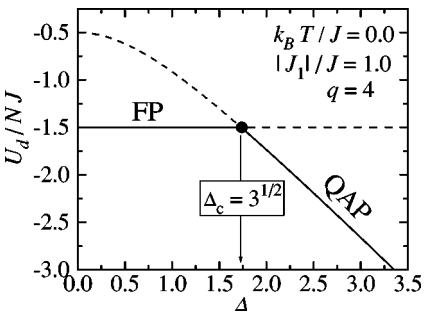

FIG. 4. Ground-state energy U_d vs Δ for $q=4$ and $|J_1|/J$ $=1.0$. The full and dashed lines represent, respectively, the stable and unstable parts of the energies of relevant phases. The black circle denotes the ground-state energy of the disordered phase (DP).

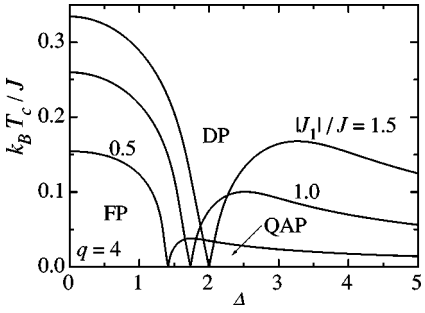

FIG. 5. Phase boundaries in the $\Delta - T_c$ plane for the doubly decorated square Ising-Heisenberg lattice ($q=4$) when the exchange interaction J_1 is changed. FP, QAP, and DP denote the ferromagnetic (or ferrimagnetic), quantum antiferromagnetic and disordered phase, respectively.

universality class as that of the usual 2D Ising model. Of course, the thermal variations of physical quantities can differ from the standard behaviors in the Ising model. To illustrate the case, we have shown in Fig. 6 the temperature dependences of the specific heat for $J_1/J=0.5$. As we can see, in the isotropic case ($\Delta=1.0$) we have the standard dependence usually observed in the Ising models. On the other hand, for the values of the exchange anisotropy close to the critical value ($\Delta_c=\sqrt{2}$), the specific heat may in addition to the familiar Schottky-type maximum exhibit another maxima. These maxima appear equally bellow (see the case $\Delta=1.3$) and above (see the inset in Fig. 6) the critical temperature, as a consequence of the thermal excitations of the Heisenberg spins that basically influence the ordering in the system. The influence of the thermal excitations on the behavior of the system is really of great importance, and can be understood from the temperature dependences of the correlation functions. For this purpose, in Figs. 7–9 we plot thermal variations of the correlations q_{ih}^{zz}, q_{hh}^{zz} and q_{hh}^{xx} for the same values of J_1 and Δ as in Fig. 6. It is clear from these figures (see the case $\Delta=1.3$) that the occurrence of the maximum bellow the critical temperature require to satisfy two conditions: (i) the relevant correlations must increase (decrease) rapidly enough with the increasing temperature in the low-temperature region (for example, in the case of $\Delta=1.0$ the additional maximum does not appear due to the relatively slow excitation process in comparison with the case of $\Delta=1.3$); and (ii) the critical temperature of the system must be relatively high (for instance, in the case of $\Delta=1.4$ we have $k_B T_c/J \approx 0.0075$ that is very low for the occurrence of the maximum below T_c, in spite of the very strong thermal excitations).

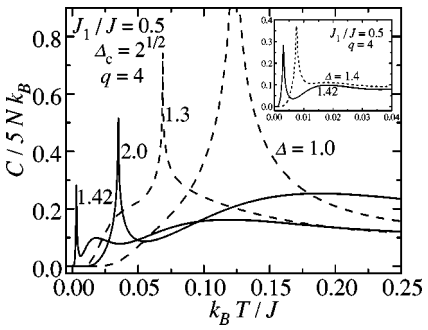

FIG. 6. Temperature dependences of the reduced specific heat of the doubly decorated square lattice ($q=4$) for $J_1/J=0.5$ and different values of the anisotropy parameter Δ. The dashed (full) lines represent the cases corresponding to the FP (QAP) ground-state phases, respectively. The inset shows the detail of the behavior when the anisotropy parameter Δ takes the value close to the boundary value $\Delta_c=\sqrt{2}$.

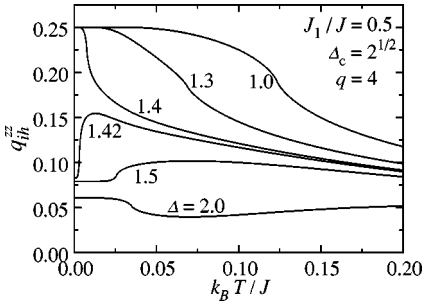

FIG. 7. Temperature variations of the correlation function q_{ih}^{zz} between Ising and Heisenberg atoms for $q=4$, $J_1/J=0.5$ and different values of the anisotropy parameter Δ.

In addition to this behavior, the double-peak specific heat curve can be also observed here. The origin of the relevant maxima above the critical temperature can be understood from the thermal dependences of the correlation functions, as it is clearly displayed in Figs. 6–9 for $\Delta=1.42$. As one can see, the correlation function q_{ih}^{zz} rapidly increases in the relevant region, though the short-range ordering of Heisenberg atoms in the *xy* plane as well as in the *z* direction is rapidly destroyed. Very similar behavior appears above T_c also for $\Delta<\Delta_c$ excepting the fact that in this case the correlations in the *xy* plane abruptly increases, although all the other correlations rapidly decreases as it is apparent from Figs. 7–9 for the case of $\Delta=1.4$. Hence the appearance of the multiple peaks in the specific heat curve arises due to the relevant thermally induced short-range ordering or disordering in the system. Finally, one should also mention that all pair-correlation function exhibit at critical temperature weak energy-type singularity known from the usual Ising models.

Although, the numerical calculation have been presented for the square lattice $q=4$, we can, on the basis of our formulation, draw some general conclusions about the behavior

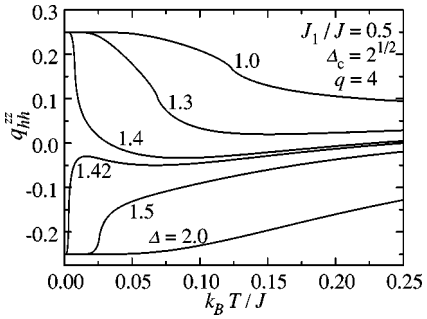

FIG. 8. The same as in Fig. 7, but for the correlation q_{hh}^{zz} between nearest-neighboring Heisenberg atoms.

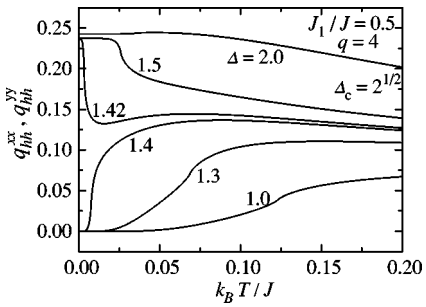

FIG. 9. The same as in Fig. 7, but for the correlation $q_{hh}^{xx}=q_{hh}^{yy}$ between nearest-neighboring Heisenberg atoms.

of the doubly decorated Ising-Heisenberg systems. However, one should emphasize that our next statements do not concern the one-dimensional case that exhibits quite different behavior, as result of the fact that no long-range order is possible in the system at nonzero temperatures.

First, it is clear from Eqs. (21)–(23) that the ground-state phase diagram does not depend on the coordination number and spatial dimensionality of the system. This implies that the value of Δ_c is also independent of the coordination number and dimension, although our preliminary investigation of the other systems has revealed that it depends on the spin value of the Heisenberg atoms. In general one can say that the QAP exists in many two- and three-dimensional lattices in the region of $\Delta>\Delta_c$. However, it is necessary to emphasize the fact that the above statement is valid only in the case when the Néel order is possible on the relevant original lattice. Apparently, this not the case, for example, for the doubly decorated triangular or Kagomé lattices, for which much more complicated phases will occur for $\Delta>\Delta_c$.

It is also interesting to note that the QAP, as well as the standard FP, may exist at finite temperatures and the temperature region of their stability is clearly enlarged with the increasing coordination number and dimensionality of the system. This is a consequence of the fact that the critical temperature increases with the increasing coordination number and dimensionality of the system. Of course, the thermal fluctuations gradually destroy the long-range order (both for the FP and QAP) in the system, and, if the temperature reaches its critical value, then the system undergoes the second-order phase transition sharing the same universality class as the standard spin-1/2 Ising planar model.

IV. CONCLUSION

In this work we have studied the doubly decorated Ising-Heisenberg model on planar lattices. Applying the standard decoration-iteration transformation, we have obtained the simple relation between the partition function of the decorated model and its corresponding standard spin-1/2 Ising model. On the basis of this relation, we have derived the exact results for basic physical quantities that have been subsequently discussed for $J>0$ in Sec. III.

In our opinion, the prediction of the QAP is the most important finding of this work, and it illustrates how the magnetic properties of the pure Ising systems can be essentially modified by introducing the quantum Heisenberg atoms on the bonds of the original lattice. The origin of the QAP consists in the quantum fluctuations arising in the system; hence the QAP itself provides a clear manifestation of the quantum phenomena in the macroscopic scale.

Although at the present time we are not aware of any experimental system which can be directly described by the considered doubly decorated Ising-Heisenberg model, we hope that the recent progress in molecular engineering will result in the preparation of such materials. In fact, recently synthesized compound $K_3Co^{III}(CN)_6.2Rh_2^{II}(CH_3COO)_4$ (see Ref. 16), which has the magnetic structure of the doubly decorated square lattice (Fig. 1), seems to be the most promising from this point of view. Unfortunately, the Co^{3+} ions (located at the corners of each square) are in this compound due to the very strong ligand field of the cyanide groups in the low-spin state (i.e. they are diamagnetic). Nevertheless, tuning the ligand field around the Co^{3+} ions by the choice of other ligands, represents a possible way how to prepare the compounds with high-spin Co^{3+} paramagnetic ions. Another possibility to obtain the compounds of desired magnetic structure consists in the chemical replacement of the Co^{3+} ions by other transition metal ions, such as Fe^{3+} and Cr^{3+} ions. Because the corner atoms of each square would possess a spin 1/2 (in case of Fe^{3+} ion) or 3/2 (for Cr^{3+} ion), the present theory could be applied to describe the behavior of these materials. Since the most of the real materials have $\Delta \approx 1$, it is also worth noticing that in the case of very weak exchange interaction J_1 ($|J_1| \ll J$), the QAP appears in our system near $\Delta \approx 1$ regardless of the coordination number and spatial dimensionality. This supports our hope that the experimental confirmation of this phase would be possible in some materials.

Finally, we would like to remark that the present formalism can be extended to investigate many other interesting systems. Indeed, we have succeeded in solving some interesting generalization of the system studied in this paper and we have found very rich and interesting behavior that will be discussed in forthcoming works.

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APPENDIX

$$K_0=\frac{1}{8}\frac{\sinh(\beta J_1/2)}{\cosh(\beta J_1/2)+\exp(-\beta J/2)\cosh(\beta J\Delta/2)},$$

$$K_1=\frac{1}{8}\frac{\sinh(\beta J\Delta/2)}{\cosh(\beta J\Delta/2)+\exp(\beta J/2)\cosh(\beta J_1/2)},$$

$$K_2=\frac{1}{8}\frac{J\Delta}{\sqrt{J_1^2+J^2\Delta^2}}\frac{\sinh(\beta\sqrt{J_1^2+J^2\Delta^2}/2)}{\cosh(\beta\sqrt{J_1^2+J^2\Delta^2}/2)+\exp(\beta J/2)},$$

$$K_3=\frac{1}{8}\frac{\cosh(\beta J_1/2)-\exp(-\beta J/2)\cosh(\beta J\Delta/2)}{\cosh(\beta J_1/2)+\exp(-\beta J/2)\cosh(\beta J\Delta/2)},$$

$$K_4=\frac{1}{8}\frac{\exp(\beta J/2)-\cosh(\beta\sqrt{J_1^2+J^2\Delta^2}/2)}{\exp(\beta J/2)+\cosh(\beta\sqrt{J_1^2+J^2\Delta^2}/2)},$$

$$K_5=\frac{1}{8}\frac{J_1}{\sqrt{J_1^2+J^2\Delta^2}}\frac{\sinh(\beta\sqrt{J_1^2+J^2\Delta^2}/2)}{\cosh(\beta\sqrt{J_1^2+J^2\Delta^2}/2)+\exp(\beta J/2)}.$$

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The detailed derivation of the coefficients given above requires a lengthy calculation, and thus is not presented here; however, it can be obtained from the authors on the request.

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