Phase transitions in exactly solvable decorated model of localized Ising spins and itinerant electrons

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Abstract. A hybrid lattice-statistical model of doubly decorated two-dimensional lattices, which have localized Ising spins at its nodal sites and itinerant electrons delocalized over decorating sites, is exactly solved with the help of a generalized decoration-iteration transformation. Under the assumption of a quarter filling of each couple of the decorating sites, the ground state constitutes either spontaneously long-range ordered ferromagnetic or ferrimagnetic phase in dependence on whether the ferromagnetic or antiferromagnetic interaction between the localized Ising spins and itinerant electrons is considered. The critical temperature of the spontaneously long-range ordered phases monotonically increases upon strengthening the ratio between the kinetic term and the Ising-type exchange interaction.

1. Introduction

Exactly soluble lattice-statistical models traditionally attract appreciable scientific interest as they offer a valuable insight into diverse aspects of cooperative phenomena [1]. It should be mentioned, however, that sophisticated mathematical methods must be usually employed when searching for an exact treatment of even relatively simple interacting many-body systems and consequently, a theoretical treatment of more realistic or more complex models is often accompanied with a substantial increase of computational difficulties. The mapping technique based on generalised algebraic transformations belongs to the simplest mathematical methods, which allow to obtain the exact solution of a more complicated model from a precise mapping relationship with a simpler exactly solved model [2-3]. Recently, this approach has been applied to an intriguing diamond chain model of interacting spin-electron system [4-5]. The purpose of this work is to treat exactly similar two-dimensional (2D) model, which should provide a deeper insight into phase transitions and critical phenomena of interacting spin-electron systems.

2. Model and its exact solution

Let us consider a hybrid lattice-statistical model of interacting spin-electron system on doubly decorated 2D lattices, which have one localized Ising spin at each nodal site and one itinerant electron delocalized over each couple of decorating sites. The magnetic structure of the model under investigation is schematically illustrated in figure 1 on the particular example of the doubly decorated square lattice. For further convenience, let us define the total Hamiltonian as
a sum over bond Hamiltonians $\mathcal{H} = \sum_k \mathcal{H}_k$, where each bond Hamiltonian $\mathcal{H}_k$ involves all the interaction terms of one itinerant electron from the $k$th couple of the decorating sites

$$
\mathcal{H}_k = -t \left( c_{k,1}^\dagger c_{k,2} + c_{k,2}^\dagger c_{k,1} + c_{k,1}^\dagger c_{k,1}^\dagger + c_{k,2}^\dagger c_{k,1} \right) - J \left[ \frac{1}{2} \left( \hat{\sigma}_{k1}^z (c_{k,1}^\dagger c_{k,1} - c_{k,1} c_{k,1}^\dagger) + \hat{\sigma}_{k2}^z (c_{k,2}^\dagger c_{k,2} - c_{k,2} c_{k,2}^\dagger) \right) \right].
$$

In above, $c_{k,\alpha,\gamma}^\dagger$ and $c_{k,\alpha,\gamma}$ ($\alpha = 1, 2$, $\gamma = \uparrow, \downarrow$) denote usual creation and annihilation fermionic operators and $\hat{\sigma}_{k\alpha}$ is the standard spin-1/2 operator with the eigenvalues $\sigma_{k\alpha} = \pm 1/2$. The transfer integral $t$ takes into account a kinetic energy of a single electron delocalized over a couple of the decorating sites and the exchange integral $J$ describes the Ising-type interaction between the delocalized electron and its two nearest-neighbouring localized Ising spins.

The crucial step of our calculation represents an evaluation of the partition function. A validity of the commutation relation between different bond Hamiltonians $[\mathcal{H}_i, \mathcal{H}_j] = 0$ allows a straightforward factorization of the total partition function $Z$ into a product performed over bond partition functions $Z_k$

$$
Z = \text{Tr}_{\{\sigma_i\}} \text{Tr}_{\{c_i\}} \exp\left( -\beta \mathcal{H} \right) = \text{Tr}_{\{\sigma_i\}} \prod_{k=1}^{Nq/2} \text{Tr}_{c_{k1},c_{k2}} \exp\left( -\beta \mathcal{H}_k \right) = \text{Tr}_{\{\sigma_i\}} \prod_{k=1}^{Nq/2} Z_k,
$$

where $\beta = 1/(k_B T)$, $k_B$ is Boltzmann’s constant, $T$ is the absolute temperature, $N$ is the total number of the Ising spins (i.e. the nodal lattice sites) and $q$ is their coordination number (i.e. the number of nearest neighbours). Next, the symbols $\text{Tr}_{\{\sigma_i\}}$ and $\text{Tr}_{\{c_i\}}$ denote a trace over degrees of freedom of all Ising spins and itinerant electrons, respectively, while the symbol $\text{Tr}_{c_{k1},c_{k2}}$ stands for a trace over degrees of freedom of the itinerant electron from the $k$th couple of decorating sites.

After the elementary diagonalisation of the bond Hamiltonian $\mathcal{H}_k$, one arrives at the explicit expression of the bond partition function $Z_k$, which can be eventually replaced through the appropriately chosen generalised decoration-iteration transformation [2, 3]

$$
Z_k = 4 \cosh \left[ \frac{\beta J}{4} (\sigma_{k1} + \sigma_{k2}^z) \right] \cosh \left[ \frac{\beta}{4} \sqrt{J^2 (\sigma_{k1}^z - \sigma_{k2}^z)^2 + (4t)^2} \right] = A \exp(\beta R \sigma_{k1}^z \sigma_{k2}^z).
$$

The 'self-consistency' condition of the algebraic transformation [3] requires that this mapping relationship must hold independently of the spin states of two Ising spins $\sigma_{k1}^z$ and $\sigma_{k2}^z$ involved therein, which directly determines so far not specified transformation parameters $A$ and $R$ as

$$
A = 4 \left\{ \cosh (\beta t) \cosh \left( \frac{\beta J}{4} \right) \cosh \left[ \frac{\beta}{4} \sqrt{J^2 + (4t)^2} \right] \right\}^{1/2}, \quad \beta R = 2 \ln \left\{ \frac{\cosh (\beta t) \cosh \left( \frac{\beta J}{4} \right)}{\cosh \left[ \frac{\beta}{4} \sqrt{J^2 + (4t)^2} \right]} \right\}.
$$
At this stage, a substitution of the generalised decoration-iteration transformation \((3)\) into Eq. \((2)\) yields in turn a simple mapping relation between the partition function of the interacting spin-electron system on the doubly decorated 2D lattice and the partition function of the simple spin-1/2 Ising model on the corresponding undecorated lattice

\[
Z(\beta, J, t) = A^{Nq/2} Z_{\text{IM}}(\beta, R).
\]  

(5)

It can be easily understood from Eqs. \((4)\) and \((5)\) that the mapping parameter \(A\) cannot cause a non-analytic behaviour of the partition function \(Z\) and hence, the investigated spin-electron system becomes critical if and only if the corresponding spin-1/2 Ising model becomes critical as well. Accordingly, the lines of critical points can readily be obtained from a comparison of the effective temperature-dependent coupling \(\beta R\) with the relevant critical points of the spin-1/2 Ising model on the corresponding undecorated lattices that are given by \(\beta_c R = 2 \ln(2 + \sqrt{3})\), \(2 \ln(1 + \sqrt{2})\), and \(\ln 3\) for the honeycomb, square, and triangular lattices \([6]\), respectively.

Other thermodynamic quantities can be now easily derived from the mapping relation \((5)\) between the partition functions. For instance, both sublattice magnetisations can be calculated by combining the mapping relation \((5)\) with the exact Callen-Suzuki identity. As a result, the sublattice magnetisations \(m_i\) and \(m_e\) per one Ising spin and per one itinerant electron read

\[
m_i = m_{\text{IM}}(\beta R), \quad m_e = \tanh(\beta J/4) m_{\text{IM}}(\beta R),
\]

(6)

where \(m_{\text{IM}}(\beta R)\) denotes the spontaneous magnetisation of the spin-1/2 Ising model on the corresponding undecorated lattice that is known for several planar lattices \([6]\).

3. Results and discussion

Let us proceed to a discussion of the most interesting results obtained in the preceding section. First, it should be realized that the effective coupling \((4)\) of the spin-1/2 Ising model on the corresponding undecorated lattice is always positive, i.e. \(\beta R > 0\), which means that the interacting spin-electron system is effectively mapped to the ferromagnetic spin-1/2 Ising model. Hence, it directly follows from Eq. \((6)\) that the ground state constitutes either the classical ferromagnetic phase with fully saturated and identically oriented sublattice magnetisations \(m_i = m_e = 1/2\) on assumption that \(J > 0\), or the classical ferrimagnetic phase with fully saturated sublattice magnetisations oriented opposite one to each other \(m_i = -m_e = 1/2\) if \(J < 0\). Both the spontaneously long-range ordered phases exhibit completely the same critical behaviour as a result of the invariance of the effective coupling \(\beta R\) with respect to the transformation \(J \rightarrow -J\).

The reduced critical temperature of the spontaneously long-range ordered phases is plotted in Fig. 2 against the ratio \(t/|J|\) between the hopping term and the exchange integral. As one can see, the critical temperature rises steadily when increasing a relative strength of the kinetic term until it asymptotically tends towards its maximum value achieved in the limit \(t/|J| \rightarrow \infty\). In the limit \(t/|J| \rightarrow 0\), the observed zero critical temperature is consistent with a non-magnetic character of one of two decorating sites on each bond of the doubly decorated lattice. On the other hand, the highest asymptotic values of the critical temperatures for the interacting spin-electron system on the doubly decorated honeycomb, square and triangular lattices

\[
\frac{k_B T_c}{J_{hc}} = \frac{1}{4 \ln(2 + \sqrt{3} + \sqrt{6} + 4\sqrt{3})}, \quad \frac{k_B T_c}{J_{sq}} = \frac{1}{4 \ln(1 + \sqrt{2} + \sqrt{2 + 2\sqrt{2}})} , \quad \frac{k_B T_c}{J_{tr}} = \frac{1}{4 \ln(\sqrt{2} + \sqrt{3})},
\]

(7)

are exactly a half of the relevant critical temperatures of the spin-1/2 Ising model on singly decorated honeycomb, square, and triangular lattices, respectively. This observation would
suggest that a delocalization of itinerant electrons generally reduces the critical temperature, because the localized Ising spins effectively feel due to the hopping process less than a half of the total magnetic moment of each itinerant electron.

Thermal variations of the total and sublattice magnetisations are displayed in Fig. 3 for three different values of a relative strength of the kinetic term. It is quite obvious from this figure that both sublattice magnetisations exhibit quite similar temperature dependencies when the sublattice magnetization \( m_i \) of the localized Ising spins lies just slightly above the sublattice magnetisation \( m_e \) of the itinerant electrons. A closer analysis reveals that both sublattice magnetisations tend to zero in a vicinity of the critical temperature with the critical exponent from the standard Ising universality class.

To conclude, we have found the exact solution for the hybrid model of the interacting spin-electron system on doubly decorated 2D lattices. Under the assumption of quarter filling of each couple of the decorating sites, the ground state constitutes either spontaneously long-range ordered ferromagnetic or ferrimagnetic phase in dependence on whether the ferromagnetic or antiferromagnetic interaction between the localized Ising spins and itinerant electrons is assumed. It has been shown that the critical temperature of spontaneously long-range ordered phases monotonically increases upon strengthening the ratio between the kinetic term and the exchange interaction. The work on an analogous 2D hybrid model of interacting spin-electron system with two electrons per each couple of the decorating sites is in progress [7].

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