Exact results of the transverse mixed spin-1/2 and spin-S_B Ising model on the honeycomb lattice

2000 J. Phys.: Condens. Matter 12 L583

(http://iopscience.iop.org/0953-8984/12/36/102)

J. Phys.: Condens. Matter **12** (2000) L583–L589. Printed in the UK PII: S0953-8984(00)15112-4

LETTER TO THE EDITOR

Exact results of the transverse mixed spin-1/2 and spin-S_B Ising model on the honeycomb lattice

Michal Jaščur and Silvia Lacková

Department of Theoretical Physics and Geophysics, Faculty of Science, P J Šafárik University, Moyzesova 16, 041 54 Košice, Slovak Republic

E-mail: jascur@kosice.upjs.sk

Received 30 June 2000, in final form 11 August 2000

Abstract. A transverse mixed spin-1/2 and spin-S_B Ising model on the honeycomb lattice is studied by the use of a generalized star-triangle transformation which maps the model on an exactly solvable Ising model. The exact results for the phase diagram, compensation temperature, magnetization and transverse susceptibility are obtained and discussed.

Exact calculations in statistical mechanics traditionally attract considerable interest of researchers since they are very important for direct comparisons with experimental data. Moreover, from the theoretical point of view they are extremely useful for testing various approximated schemes. Very nice and clear exposition of the exactly solved models can be found in the book by Baxter [1]. It is well known, that the straightforward exact treatment of the two- and three-dimensional models is very hard and requires extraordinary mathematical skills. A simpler way for obtaining exact results (which is also used in this work) is based on the mapping of a new model on the relevant exactly solvable model [2].

In this article, we will deal with the transverse Ising model which has been recently intensively studied both experimentally and theoretically. From the experimental point of view, the transverse Ising model is a valuable model because of its applications, for example in studies of hydrogen bonded ferroelectrics [3], cooperative Jahn-Teller systems [4] and strongly anisotropic magnetic materials in the transverse field [5]. More details about possible applications of the model can be found in reviews of Blinc and Zeks [6] and Stinchcombe [7]. Although the transverse Ising model is one of the simplest quantum models, the complete exact solutions have been obtained only in the one-dimensional case [8]. For two-dimensional systems the exact results are known only for the initial transverse susceptibility on regular lattices [9].

In general, the main mathematical problem in treating quantum statistical models (including the transverse Ising model) is the noncommutability of relevant operators in the Hamiltonian. To overcome this difficulty, we introduce in the present paper a transverse Ising model on the honeycomb lattice consisting of classical (Ising-type) and quantal spins which can be exactly solved by the use of generalized star-triangle transformation [10].

In what follows, we will study the two-sublattice mixed spin ($S_A = 1/2$, $S_B > 1/2$) Ising system on the honeycomb lattice in which only spins on the sublattice B interact with the transverse field. The Hamiltonian of the system can be written in the form

$$\hat{\mathcal{H}}_h = \sum_i \hat{\mathcal{H}}_i \tag{1}$$

with $\hat{\mathcal{H}}_i = -J(\hat{\mu}_{i1}^z + \hat{\mu}_{i2}^z + \hat{\mu}_{i3}^z)\hat{S}_i^z - \Omega\hat{S}_i^x$, where the summation is over all sites of sublattice B. The classical Ising spins $\hat{\mu}_{ik}$ occupy sublattice A and the quantum spins $\hat{S}_i$ occupy sublattice B. The first term of the site Hamiltonian $\mathcal{H}_i$ describes the interaction of the B atom with its three nearest-neighbours and the second one expresses the interaction of B atom with the transverse field (Ω). It is worth noticing that the ground state of our system orders ferromagnetically for $J > 0$ or ferrimagnetically for $J < 0$.

Owing to the topology of the lattice, the site Hamiltonian $\hat{\mathcal{H}}_i$ obeys the following commutation relation

$$[\hat{\mathcal{H}}_i, \hat{\mathcal{H}}_j] = 0 \qquad i \neq j \tag{2}$$

which is of principal importance to ensure exact solvability of the model under investigation. The partition function of the system takes the form

$$\mathcal{Z}_h = \mathrm{Tr}\,\mathrm{e}^{-\beta\hat{\mathcal{H}}_h} = \mathrm{Tr}\prod_{i=1}^{N/2}\mathrm{e}^{-\beta\hat{\mathcal{H}}_i} \tag{3}$$

where N denotes the total number of atoms on the honeycomb lattice and $\beta = 1/k_BT$. To proceed further, one now has to diagonalize the site Hamiltonian $\hat{\mathcal{H}}_i$. Fortunately, it can be directly performed by using the following rotational transformation

$$\hat{S}_i^z = \hat{S}_i^{z'}\cos(\varphi_i) - \hat{S}_i^{x'}\sin(\varphi_i) \qquad \hat{S}_i^x = \hat{S}_i^{z'}\sin(\varphi_i) + \hat{S}_i^{x'}\cos(\varphi_i) \tag{4}$$

where

$$\sin(\varphi_i) = \frac{\Omega}{\sqrt{\Omega^2 + \Theta_i^2}} \qquad \cos(\varphi_i) = \frac{\Theta_i}{\sqrt{\Omega^2 + \Theta_i^2}} \qquad \text{and} \qquad \Theta_i = J(\hat{\mu}_{i1}^z + \hat{\mu}_{i2}^z + \hat{\mu}_{i3}^z). \tag{5}$$

Applying relations (4)–(5) we can rewrite equation (3) as follows

$$\mathcal{Z}_h = \sum_{\{\mu_{\alpha i}^z\}}\prod_{i=1}^{N/2}\sum_{S_i^{z'}}\exp\left\{S_i^{z'}\beta\sqrt{\Omega^2 + [J(\mu_{i1}^z + \mu_{i2}^z + \mu_{i3}^z)]^2}\right\} \tag{6}$$

where $\sum_{S_i^{z'}}$ runs over $(2S_B + 1)$ possible states of the B atom residing on the ith site and $\sum_{\{\mu_{i\alpha}^z\}}$ (with $\mu_{i\alpha}^z = \pm 1/2$) represents the trace over all possible configurations of A atoms. The form of equation (6) implies the possibility to introduce following generalized star-triangle (or $Y - \Delta$) transformation

$$\sum_{S_i^{z'}=-S_B}^{S_B}\exp\left\{S_i^{z'}\beta\sqrt{\Omega^2 + [J(\mu_{i1}^z + \mu_{i2}^z + \mu_{i3}^z)]^2}\right\} = A\exp\left\{\beta R(\mu_{i1}^z\mu_{i2}^z + \mu_{i2}^z\mu_{i3}^z + \mu_{i1}^z\mu_{i3}^z)\right\}. \tag{7}$$

Here A and R stand for unknown parameters (R being the exchange parameter of the relevant triangular lattice) that can be expressed in the form (see for example [10])

$$A^4 = V_1V_2^3 \qquad \beta R = \ln\frac{V_1}{V_2} \tag{8}$$

where we have defined the functions

$$V_1 = \sum_{n=-S_B}^{S_B}\cosh\left(\frac{n\beta}{2}\sqrt{9J^2 + 4\Omega^2}\right) \qquad V_2 = \sum_{n=-S_B}^{S_B}\cosh\left(\frac{n\beta}{2}\sqrt{J^2 + 4\Omega^2}\right). \tag{9}$$

Now, after putting the critical temperature of the triangular lattice ($\beta_c R = R/k_B T_c = \ln 3$) into equation (8), we obtain the following equation for the critical temperature of our system

$$\sum_{n=-S_B}^{S_B} \left\{ 3\cosh\left(\frac{n\beta_c}{2}\sqrt{J^2+4\Omega^2}\right) - \cosh\left(\frac{n\beta_c}{2}\sqrt{9J^2+4\Omega^2}\right) \right\} = 0 \qquad \beta_c = 1/k_B T_c. \quad (10)$$

From this equation one can find the transverse-field dependences of the critical temperature for arbitrary values of the spin S_B.

To make a progress in calculating other physical quantities, we substitute equation (7) into equation (6) and obtain relation

$$\mathcal{Z}_h(J, T, \Omega) = A^{\frac{N}{2}} \mathcal{Z}_t(R, T) \quad (11)$$

which relates the partition function of the transverse Ising model on the honeycomb lattice ($\mathcal{Z}_h$) to that of the standard spin-1/2 Ising model on the triangular lattice ($\mathcal{Z}_t$). The parameters A and R obviously satisfy equation (8). One should notice that the transformation (8) is rather general since it is valid for arbitrary spin values S_B, however, it is limited topologically. In principle, from equation (11) one can obtain some physical quantities (such as the free energy, internal energy, transverse magnetization and specific heat) by exploring familiar thermodynamic relations. Nevertheless, in practice the calculations are extremely tedious and complicated because of elliptic integrals included in the exact relations for the relevant quantities of the triangular lattice. Another problem appearing in this approach is that we cannot determine the longitudinal magnetization which is very important for understanding the magnetic properties of the system. For this reason, we will now explain an alternative way to avoid the above mentioned problems.

First of all, we will study the magnetization of our system. As mentioned above, the honeycomb lattice consists of two interpenetrating sublattices with different spins, thus the sublattice magnetization must be treated separately. The starting point for our calculation is the Callen–Suzuki-type identity

$$\langle (\hat{S}_i^\alpha)^k \rangle_h = \left\langle \frac{\mathrm{Tr}_i[(\hat{S}_i^\alpha)^k \exp(-\beta \hat{\mathcal{H}}_i)]}{\mathrm{Tr}_i \exp(-\beta \hat{\mathcal{H}}_i)} \right\rangle_h \qquad k = 1, 2 \qquad \alpha = x, z \quad (12)$$

which can be simply derived with the help of equation (2). Here $\langle \ldots \rangle_h$ denotes the standard ensemble average calculated with the Hamiltonian (1). Now, taking into account the symmetry of the honeycomb lattice and applying one of the standard procedures (for instance, the differential operator technique [11]), we get the following exact relations for the longitudinal and transverse sublattice magnetization:

$$\begin{aligned} m_{Bh}^z &\equiv \langle \hat{S}_i^z \rangle_h = 6K_1 \langle \hat{\mu}_{i1} \rangle_h + 8K_3 \langle \hat{\mu}_{i1}^z \hat{\mu}_{i2}^z \hat{\mu}_{i3}^z \rangle_h \\ m_{Bh}^x &\equiv \langle \hat{S}_i^x \rangle_h = K_0 + 12K_2 \langle \hat{\mu}_{i1}^z \hat{\mu}_{i2}^z \rangle_h \end{aligned} \quad (13)$$

where the coefficients K_0–K_3 are given by:

$$\begin{aligned} K_0 &= \tfrac{1}{4}[G_{S_B}(3J/2) + 3G_{S_B}(J/2)] \qquad & K_1 &= \tfrac{1}{4}[F_{S_B}(3J/2) + F_{S_B}(J/2)] \\ K_2 &= \tfrac{1}{4}[G_{S_B}(3J/2) - G_{S_B}(J/2)] \qquad & K_3 &= \tfrac{1}{4}[F_{S_B}(3J/2) - 3F_{S_B}(J/2)]. \end{aligned} \quad (14)$$

The functions $F_{S_B} = x\mathcal{K}(x)$ and $G_{S_B} = \Omega\mathcal{K}(x)$ with

$$\mathcal{K}(x) = \frac{1}{\sqrt{x^2+\Omega^2}} \frac{\sum_{n=-S_B}^{S_B} n \sinh\left(n\beta\sqrt{x^2+\Omega^2}\right)}{\sum_{n=-S_B}^{S_B} \cosh\left(n\beta\sqrt{x^2+\Omega^2}\right)}. \quad (15)$$

Similarly, for $k = 2$ we obtain from equation (12) the following relation for the parameter $q^z_{Bh} \equiv \langle(\hat{S}^z_i)^2\rangle_h$

$$q^z_{Bh} = L_0 + 12L_2\langle\hat{\mu}^z_{i1}\hat{\mu}^z_{i2}\rangle_h \tag{16}$$

with

$$L_0 = \tfrac{1}{4}[H_{S_B}(3J/2) + 3H_{S_B}(J/2)] \qquad L_2 = \tfrac{1}{4}[H_{S_B}(3J/2) - H_{S_B}(J/2)]. \tag{17}$$

The function H_{S_B} also depends on the spin value S_B, and for example in the case of $S_B = 1$ is given by

$$H_1(x) = \frac{\Omega^2 + (2x^2 + \Omega^2)\cosh\beta\sqrt{x^2+\Omega^2}}{(x^2+\Omega^2)\left[2\cosh\beta\sqrt{x^2+\Omega^2} + 1\right]}. \tag{18}$$

To finish our calculations, we have to determine the spin correlations on the r.h.s of equations (13) and (16). For this purpose one can use the relation

$$\langle f(\hat{\mu}_{ij},\ \hat{\mu}_{ik}, \ldots, \hat{\mu}_{i\ell})\rangle_h = \langle f(\hat{\mu}_{ij}, \hat{\mu}_{ik}, \ldots, \hat{\mu}_{i\ell})\rangle_t \tag{19}$$

which can be straightforwardly proved from the definition with the help of equation (7). Here f stands for an arbitrary function and the symbols $\langle\ldots\rangle_h$ and $\langle\ldots\rangle_t$ denote the ensemble average on the honeycomb and triangular lattice, respectively. Consequently, from equation (19) one obtains relations

$$m_{Ah} \equiv \langle\hat{\mu}_{i1}\rangle_h = \langle\hat{\mu}_{i1}\rangle_t \qquad \langle\hat{\mu}_{i1}\hat{\mu}_{i2}\rangle_h = \langle\hat{\mu}_{i1}\hat{\mu}_{i2}\rangle_t \qquad \langle\hat{\mu}_{i1}\hat{\mu}_{i2}\hat{\mu}_{i3}\rangle_h = \langle\hat{\mu}_{i1}\hat{\mu}_{i2}\hat{\mu}_{i3}\rangle_t \tag{20}$$

that complete our calculations, since the relevant spin correlations on the triangular lattice are well known [12]. The total longitudinal magnetization of the system is then given by $M = (m^z_{Ah} + m^z_{Bh})/2$. Moreover, from the condition $M = 0$ one can calculate the compensation temperature (T_k) for the ferrimagnetic system ($J < 0$). We recall that T_k is defined as a temperature at which the total longitudinal magnetization of the system vanishes below the critical temperature (T_c). Hence, the compensation temperature can be obtained from the equation

$$1 - 6K_1 - 8K_3\frac{\langle\hat{\mu}^z_{i1}\hat{\mu}^z_{i2}\hat{\mu}^z_{i3}\rangle_h}{m_{Ah}} = 0. \tag{21}$$

It is clear from this equation that the compensation temperature will depend on the value of spin S_B as well as on the value of the transverse field Ω. Apart from the quantities discussed above, we are also able to get the transverse susceptibility which is defined as follows

$$\chi_\perp = \left(\frac{\partial M^x_{Bh}}{\partial\Omega}\right)_T = \frac{N}{2}\left(\frac{\partial m^x_{Bh}}{\partial\Omega}\right)_T. \tag{22}$$

Finally, the internal energy can be found from the relation

$$U_h \equiv \langle\hat{\mathcal{H}}_h\rangle_h = -\frac{3NJ}{2}\langle\hat{S}^z_i\hat{\mu}^z_{i1}\rangle_h - \frac{N\Omega}{2}\langle\hat{S}^x_i\rangle_h \tag{23}$$

where $\langle\hat{S}^z_i\hat{\mu}^z_{i1}\rangle_h = (K_1/2) + (4K_1 + 2K_3)\langle\hat{\mu}^z_{i1}\hat{\mu}^z_{i2}\rangle_h$ and $\langle\hat{S}^x_i\rangle_h$ is given by (13).

Now, let us discuss some interesting numerical results for the system under investigation. At first, shown in figure 1 are the phase diagrams in the $\Omega{-}T_c$ plane for $S_B = 1, 3/2$ and 2. It can be seen from the figure that the critical temperature monotonically decreases from its maximum value at $\Omega = 0$ and tends to zero for $\Omega \to \infty$. These results are qualitatively very similar to those found in randomly diluted transverse Ising systems [13]. We recall that in the standard models where all of the spins interact with the transverse field there exists a critical value of the transverse field above which the ground state of the system becomes disordered. We can see that the behaviour of our system differs from the standard picture since the ground state of our

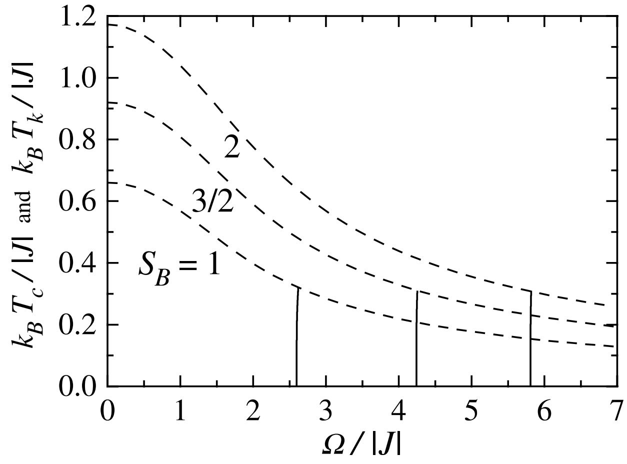

Figure 1. Transverse-field dependences of the critical (dashed lines) and compensation (solid lines) temperatures for the transverse mixed spin Ising model on the honeycomb lattice.

system remains ordered regardless of the value of the transverse field. This behaviour is caused by the presence of Ising-type A atoms in the system that do not interact with the transverse field. One should also notice that the phase diagrams are the same for both ferromagnetic and ferrimagnetic systems, since equation (10) is invariant under transformation $J = -J$. In addition to the critical temperature, we have also investigated the transverse-field dependences of the compensation temperature, that are depicted by solid lines in figure 1. We have observed that the compensation temperatures decrease with decreasing value of Ω and reduce to zero at a certain critical value which is given by $\Omega_0/|J| = 3(\sqrt{4S_B^2 - 1})/2$. We can also see that the region where the compensation effect appears is very narrow ($\Delta\Omega_k/|J| \approx 0.1 - 0.2$) and moves to higher values of Ω with the increasing value of the spin S_B.

Next, let us discuss the temperature dependences of the longitudinal and transverse magnetization. Here it is worth noticing that the magnetization exhibit qualitatively very similar behaviour for the systems with different spin S_B. For this reason we restrict our attention to the case of $S_B = 1$ only and we will consider the ferrimagnetic case which is more interesting than ferromagnetic one. In figures 2 and 3, the temperature dependences of the total longitudinal (M) and transverse magnetization m_{Bh}^x are depicted for some typical

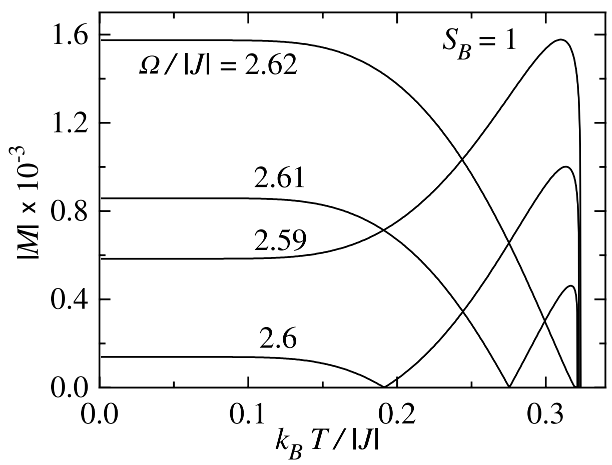

Figure 2. Longitudinal magnetization curves of the transverse mixed spin-1/2 and spin-1 Ising model on the honeycomb lattice.

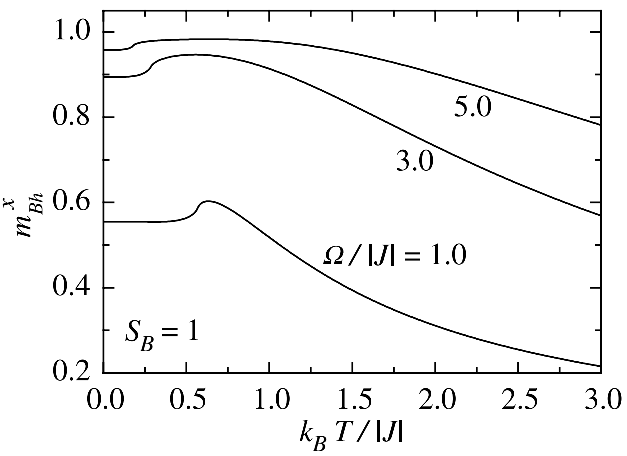

Figure 3. Temperature dependences of the transverse magnetization for the transverse mixed spin-1/2 and spin-1 Ising model on the honeycomb lattice.

values of the transverse field Ω. We can see that by applying the transverse field, the effect of compensation is really induced in the system. This phenomenon appears because of the different influence of the transverse field on the sublattice A and B, respectively. One should also notice that the critical behaviour of the system is universal i.e. the system belongs to the same universality class as the usual two-dimensional Ising model. The results in figure 3 for the transverse sublattice magnetization curves m_{Bh}^x exhibit completely different behaviour since the magnetization in the x direction exists at all temperatures (for $\Omega \neq 0$).

In conclusion, we have studied in this work the transverse mixed spin Ising model which is exactly solvable by the use of the generalized star-triangle transformation. We have investigated the phase diagrams and the compensation temperatures of the system for the case of $S_B = 1$, $3/2$ and 2. In addition, we have also studied other physical quantities such as the longitudinal and transverse magnetization. It is clear that the method presented in this work can be naturally extended to other planar lattices that satisfy topological requirements following from the generalized star-triangle transformation.

This work has been supported by the Ministry of Education of Slovak Republic under grant No. 1/6020/99.

References

[1] Baxter R J 1982 *Exactly solved models in Statistical Mechanics* (New York: Academic Press)
[2] Dembinski S T and Wydro T 1975 *Phys. Status. Solidi* b **67** K123
Blöte H W J 1979 *J. Appl. Phys.* **50** 7401
[3] de Gennes P G 1963 *Solid State Commun.* **1** 132
[4] Elliot R J, Gehring G A, Malogemoff A P, Smith S R P, Staude N S and Tyte R N 1971 *J. Phys. C: Solid State Phys.* **4** L179
[5] Wang Y L and Cooper B 1968 *Phys. Rev.* **173** 539
[6] Blinc R and Zeks B 1972 *Adv. Phys.* **1** 693
[7] Stinchcombe R B 1973 *J. Phys. C: Solid State Phys.* **6** 2459
[8] Katsura S 1962 *Phys. Rev.* **127** 1508 Pfeuty P 1970 *Ann. Phys.* **57** 79
Grest G S and Rajagopal A K 1974 *J. Math. Phys.* **15** 589
Suzuki M 1973 *Prog. Theor. Phys.* **56** 3009
Chatterjee I 1985 *J. Phys.* C **18** L1097
Idogaki T, Rikitoku M and Tucker J W 1996 *J. Magn. Magn. Mater.* **152** 311
[9] Fisher M E 1963 *J. Math Phys.* **4** 124
Allan G A T and Bets D D 1968 *Can. J. Phys.* **46** 15

Barry J H and Kathun M 1987 *Phys. Rev.* B **35** 8601
[10] Syozi I 1951 *Prog. Theor. Phys.* **6** 306
Fisher M E 1959 *Phys. Rev.* B **113** 969
Syozi I 1972 *Phase Transitions and Critical Phenomena* ed C Domb and M S Green (New York: Academic Press) Vol 1 p 269
[11] Honmura R and Kaneyoshi T 1979 *J. Phys. C: Solid State Phys.* **12** 3979
[12] Domb C 1960 *Adv. Phys.* **9** 199
[13] Cassol T F, Figueiredo W and Plascak J A 1991 *Phys. Lett.* A **160** 518
Benayad N, Zerhouni R, Klümper A and Zittarz J 1999 *Physica* A **269** 483