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Ground state properties of a spin-3/2 model on a decorated square lattice*

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Abstract. We present the construction of an optimum ground state for a quantum spin-3/2 antiferromagnet. The spins reside on a decorated square lattice, in which the basis consists of a plaquette of four sites. By using the vertex state model approach we generate the ground state from the same vertices as those used for the corresponding ground state on the hexagonal lattice. The properties of these two ground states are very similar. Particularly there is also a parameter-controlled phase transition from a disordered to a Néel ordered phase. In the regime of this transition, ground state properties can be obtained from an integrable classical vertex model.

PACS. 75.10.Jm Quantized spin models – 05.50.+q Lattice theory and statistics (Ising, Potts, etc.)

Various kinds of applications have emerged for the *matrix product* and *vertex state model* techniques. These methods can be used to construct exact ground states for special Hamiltonians [1–4], exact stationary states for stochastic models [5,6], and variational ground states for generic Hamiltonians. The latter application is related to the *density matrix renormalization group* (DMRG) technique [7–11].

In [3] we have discussed the construction of an optimum ground state for a spin-3/2 antiferromagnet on the hexagonal lattice in detail. The ground state is given in terms of a vertex state model which contains a continuous parameter a. The calculation of ground state properties has been reduced to the solution of a two-dimensional classical vertex model. The system exhibits a second order quantum phase transition which is controlled by the anisotropy parameter a. For $a^2 < a_c^2$, $a_c^2 \approx 6.46$, correlation functions decay exponentially, for $a^2 > a_c^2$ they are of Néel type. In the regime of the phase transition the classical vertex model can be reduced to a simpler, free-fermion vertex model in good approximation.

For a quantum spin-3/2 antiferromagnet on the decorated square lattice shown in Figure 1 a vertex state model can be constructed which is completely analogous to the one presented in [3]. An antiferromagnetic spin-1/2 Heisenberg model on this lattice has been investigated in [12]. The lattice shares the following properties with the hexagonal lattice:

– It is bipartite, as indicated by the filled and unfilled circles in Figure 1.
– The coordination number is 3.

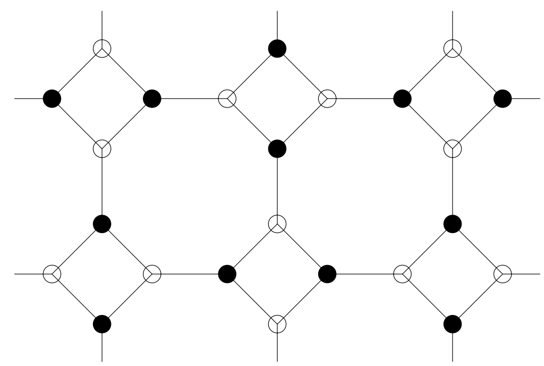

Fig. 1. The decorated square lattice. Each site of a regular square lattice is replaced by a plaquette of four spin-3/2 sites.

Therefore we can place the same vertices as in [3] (see Eq. (11) therein) on the lattice sites. This set of vertices contains the abovementioned anisotropy parameter $a \in \mathcal{R}$ and a discrete parameter $\sigma = \pm 1$. The global state $|\Psi_0\rangle$ which is generated by these vertices is antiferromagnetic in the sense that the sublattice magnetization vanishes for all values of a and σ. It is an optimum ground state of the Hamiltonian

$$H = \sum_{\langle i,j \rangle} h_{ij}, \tag{1}$$

i.e. it is also a ground state of each local interaction operator h_{ij}. This nearest-neigbour interaction is exactly the same as in the hexagonal lattice case[1].

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[1] It is constructed such that it annihilates all concatenations of adjacent vertices.

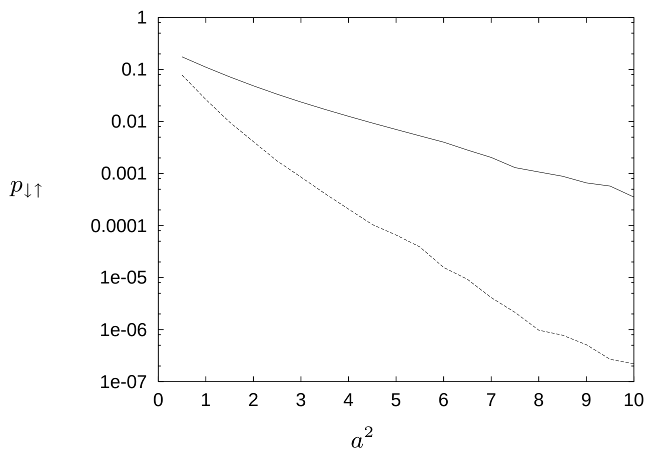

Fig. 2. Probability $p_{\downarrow\uparrow}$ for finding an antiparallel arrow pair on a bond within a plaquette (solid) and between two plaquettes (dashed).

In order to calculate properties of the vertex state model we investigate the inner product $\langle\Psi_0|\Psi_0\rangle$. As explained in [3] this inner product is given by the partition function of a classical vertex model with *two* arrow variables between each pair of adjacent sites. Motivated by the results on the hexagonal lattice we have measured numerically the probability $p_{\downarrow\uparrow}$ for finding an antiparallel arrow pair on a bond. As shown in Figure 2, $p_{\downarrow\uparrow}$ decays exponentially as a function of a^2, but for bonds within a plaquette the decay is slower than between two plaquettes. Numerically we have also found a second order phase transition at $a_c^2 \approx 7.0$. In this regime $p_{\downarrow\uparrow} \approx 0.002$, hence we neglect all vertices with antiparallel arrow pairs in the following consideration, *i.e.* we reduce the model to a vertex model with only eight different classical vertices at each site.

The next step is to sum out the four interior bonds on each plaquette, which yields a 16-vertex model on the square lattice. The vertex weights are invariant under a simultaneous flip of all four arrows, *i.e.* the model is field-free. Thus we can transform this 16-vertex model to an 8-vertex model by attaching the orthogonal 2×2-matrix

$$u = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \tag{2}$$

to each bond. If the usual notation for the 8-vertex model is used, the resulting vertex weights are

$$\begin{aligned} \omega_1 &= \tfrac{1}{2}\left(41 + 52\,a^2 + 30\,a^4 + 4\,a^6 + a^8\right) \\ \omega_2 &= \tfrac{1}{2}\left(-1 + a^2\right)^4 \\ \omega_3 = \omega_4 &= -\tfrac{1}{2}\left(-1 + a^2\right)^3\left(3 + a^2\right) \\ \omega_5 = \omega_6 &= \tfrac{1}{2}\left(-1 + a^2\right)^2\left(5 + 2\,a^2 + a^4\right) \\ \omega_7 = \omega_8 &= -\tfrac{1}{2}\left(-1 + a^2\right)^2\left(5 + 2\,a^2 + a^4\right). \end{aligned} \tag{3}$$

As in the case of the corresponding model on the hexagonal lattice, these weights fulfil the free-fermion condition

$$\omega_1\omega_2 + \omega_3\omega_4 = \omega_5\omega_6 + \omega_7\omega_8 \tag{4}$$

for all values of a, *i.e.* the model is exactly solvable.

In order to determine the phase transition point(s) of the model we investigate directly the general partition function of a free-fermionic 8-vertex model given in [13]

$$\begin{aligned} \ln Z = \frac{1}{8\pi^2}\int_0^{2\pi}\int_0^{2\pi} \ln\,[2p + 2q_1\cos\theta + 2q_2\cos\phi \\ +2q_3\cos(\theta-\phi) + 2q_4\cos(\theta+\phi)]\,\mathrm{d}\theta\,\mathrm{d}\phi, \end{aligned} \tag{5}$$

where

$$\begin{aligned} p &= \tfrac{1}{2}(\omega_1^2 + \omega_2^2 + \omega_3^2 + \omega_4^2) \\ q_1 &= \omega_1\omega_3 - \omega_2\omega_4 \\ q_2 &= \omega_1\omega_4 - \omega_2\omega_3 \\ q_3 &= \omega_3\omega_4 - \omega_7\omega_8 \\ q_4 &= \omega_3\omega_4 - \omega_5\omega_6. \end{aligned} \tag{6}$$

In case of our special set of vertex weights we have $q_1 = q_2$ and $q_3 = q_4$. This simplifies the partition function to

$$\begin{aligned} \ln Z = \frac{1}{8\pi^2}\int_0^{2\pi}\int_0^{2\pi} \ln[2p + 2q_1(\cos\theta + \cos\phi) \\ + 4q_3\cos\theta\,\cos\phi]\mathrm{d}\theta\,\mathrm{d}\phi. \end{aligned} \tag{7}$$

As explained in [13] the θ-integration can be performed by rewriting (7) in the following form

$$\ln Z = \frac{1}{8\pi^2}\int_0^{2\pi}\int_0^{2\pi} \ln\,[2A + 2B\cos\theta]\,\mathrm{d}\theta\,\mathrm{d}\phi \tag{8}$$

$$= \frac{1}{4\pi}\int_0^{2\pi} \ln\left[A + \sqrt{Q(\phi)}\right]\mathrm{d}\phi, \tag{9}$$

where

$$A = p + q_1\cos\phi,\ B = q_1 + 2q_3\cos\phi,\ Q(\phi) = A^2 - B^2. \tag{10}$$

Now we can follow the argument given in [13]. By explicitly calculating the function $Q(\phi)$ in terms of the model parameter a we observe that it is not a complete square, so (9) is analytic unless

$$Q(\phi) = 0. \tag{11}$$

The only real non-negative solution of this equation is

$$\phi_c = 0 \quad \text{and} \quad a_c^2 = 1 + \sqrt{2} + \sqrt{2(5 + 4\sqrt{2})} \approx 7.03. \tag{12}$$

This is consistent with our numerical result.

The phase transition is of the same type as in [3]. It corresponds to two simultaneous Ising transitions from a disordered phase ($a^2 < a_c^2$) with exponentially decaying correlation functions to a Néel ordered phase ($a^2 > a_c^2$) with alternating long-range correlations.

In summary we have applied the vertex state model approach to a spin-3/2 antiferromagnet on a decorated square lattice. The local interaction and the vertices used for the vertex state model are the same as those used in [3] on the hexagonal lattice. As a function of the anisotropy parameter the resulting global ground state exhibits a second order transition from a disordered phase to a Néel ordered phase. The phase transition corresponds to two simultaneous Ising transitions.

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