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Ground state phase diagram of a spin-2 antiferromagnet on the square lattice*

H. Niggemann[a], A. Klümper, and J. Zittartz

Institut für Theoretische Physik, Zülpicher Strasse 77, 50937 Köln, Germany

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Abstract. We use the vertex state model approach to construct optimum ground states for a large class of quantum spin-2 antiferromagnets on the square lattice. Optimum ground states are exact ground states of the model which minimize all local interaction operators. The ground state contains two continuous parameters and exhibits a second order phase transition from a disordered phase with exponentially decaying correlation functions to a Néel ordered phase. The behaviour is very similar to that of the corresponding ground state of a quantum spin-3/2 model on the hexagonal lattice, which has been investigated in an earlier paper.

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

1 Introduction

The matrix product technique has found a large number of applications in many particle physics. They are natural realizations of so-called *optimum ground states* for one-dimensional quantum spin models [1–3] and of stationary states for one-dimensional stochastic models [4,5]. The *vertex state model* approach used in this work is a generalization of the matrix product technique to more complicated lattice types [6,7].

As explained in [8–10] there is a connection between the matrix product technique and the *density matrix renormalization group* (DMRG) method [11]. The ground state corresponding to the fixed point of the DMRG procedure has a matrix product structure. The significance of the vertex state model approach with regard to a generalization of the DMRG method to higher dimensions is discussed in [12]. Further information about the DMRG method and its relations to the matrix product approach and other methods can be found in [13].

In this paper we consider a quantum spin-2 model on the square lattice with nearest neighbour interaction

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

The operator h_{ij} is the same on all bonds. Normalizing the energy such that the lowest eigenvalue of each h_{ij} is zero yields the equivalence

$$H|\Psi_0\rangle = 0 \quad \Longleftrightarrow \quad h_{ij}|\Psi_0\rangle = 0 \quad \text{for all nearest neighbours } i \text{ and } j. \tag{2}$$

If such a global state $|\Psi_0\rangle$ exists we call it an *optimum ground state* since the global ground state energy E_0 takes the lowest possible value. The r.h.s. of (2) can be used to find local conditions for the existence of an optimum ground state and its realization in terms of a vertex state model.

In the following we shall follow closely the procedure presented in [6], where the construction of a vertex state model for an antiferromagnetic spin-$\frac{3}{2}$ model on the hexagonal lattice is explained in detail. Section 2 contains a parametrization of all spin-2 nearest neighbour interactions which obey a certain set of symmetries. In Section 3 we present the vertices which are used to construct the global ground state. The corresponding ground state conditions are given in terms of the parameters of the general local interaction operator. Properties of the global Hamiltonian are investigated in Section 4. In particular we report on a second order quantum phase transition, which has also been found in the case of the hexagonal lattice [6]. Section 5 contains a short conclusion.

2 Parametrization of nearest-neighbour interactions

The local interaction operator h_{ij} is supposed to have at least the following symmetries:

1) parity invariance, *i.e.* $[h_{ij}, P_{ij}] = 0$, where P_{ij} is the operator which exchanges the spins at lattice sites i and j;

* Work performed within the research program of the Sonderforschungsbereich 341, Köln-Aachen-Jülich, Germany.

[a] e-mail: hn@thp.uni-koeln.de

2) rotational invariance in the xy-plane of spin space, *i.e.* $[h_{ij}, S_i^z + S_j^z] = 0$;
3) spin-flip invariance, *i.e.* h_{ij} is invariant under the transformation $S^z \to -S^z$.

In order to find a parametrization of *all* local interaction operators which fulfill the above set of symmetries we write down the general form of the simultaneous eigenstates of $S_i^z + S_j^z$ (eigenvalue $\mathfrak{m}$) and P_{ij} (eigenvalue $\mathfrak{p}$)

$$\begin{aligned}
\mathfrak{m} = \ \ 4, \mathfrak{p} = \ \ 1, |v_4\rangle \ &= |22\rangle \\
\mathfrak{m} = -4, \mathfrak{p} = \ \ 1, |v_{-4}\rangle \ &= |\overline{22}\rangle \\
\mathfrak{m} = \ \ 3, \mathfrak{p} = \ \ 1, |v_3^+\rangle \ &= |12\rangle + |21\rangle \\
\mathfrak{p} = -1, |v_3^-\rangle \ &= |12\rangle - |21\rangle \\
\mathfrak{m} = -3, \mathfrak{p} = \ \ 1, |v_{-3}^+\rangle \ &= |\overline{12}\rangle + |\overline{21}\rangle \\
\mathfrak{p} = -1, |v_{-3}^-\rangle \ &= |\overline{12}\rangle - |\overline{21}\rangle \\
\mathfrak{m} = \ \ 2, \mathfrak{p} = \ \ 1, |v_{21}^+\rangle \ &= |11\rangle + \tfrac{A}{2}(|02\rangle + |20\rangle) \\
|v_{22}^+\rangle \ &= A|11\rangle - (|02\rangle + |20\rangle) \\
\mathfrak{p} = -1, |v_2^-\rangle \ &= |02\rangle - |20\rangle \\
\mathfrak{m} = -2, \mathfrak{p} = \ \ 1, |v_{-21}^+\rangle \ &= |\overline{11}\rangle + \tfrac{A}{2}(|0\overline{2}\rangle + |\overline{2}0\rangle) \\
|v_{-22}^+\rangle \ &= A|\overline{11}\rangle - (|0\overline{2}\rangle + |\overline{2}0\rangle) \\
\mathfrak{p} = -1, |v_{-2}^-\rangle \ &= |0\overline{2}\rangle - |\overline{2}0\rangle \\
\mathfrak{m} = \ \ 1, \mathfrak{p} = \ \ 1, |v_{11}^+\rangle \ &= (|01\rangle + |10\rangle) + B(|\overline{1}2\rangle + |2\overline{1}\rangle) \\
|v_{12}^+\rangle \ &= B(|01\rangle + |10\rangle) - (|\overline{1}2\rangle + |2\overline{1}\rangle) \\
\mathfrak{p} = -1, |v_{11}^-\rangle \ &= (|01\rangle - |10\rangle) + C(|\overline{1}2\rangle - |2\overline{1}\rangle) \\
|v_{12}^-\rangle \ &= C(|01\rangle - |10\rangle) - (|\overline{1}2\rangle - |2\overline{1}\rangle) \\
\mathfrak{m} = -1, \mathfrak{p} = \ \ 1, |v_{-11}^+\rangle \ &= (|0\overline{1}\rangle + |\overline{1}0\rangle) + B(|1\overline{2}\rangle + |\overline{2}1\rangle) \\
|v_{-12}^+\rangle \ &= B(|0\overline{1}\rangle + |\overline{1}0\rangle) - (|1\overline{2}\rangle + |\overline{2}1\rangle) \\
\mathfrak{p} = -1, |v_{-11}^-\rangle \ &= (|0\overline{1}\rangle - |\overline{1}0\rangle) + C(|1\overline{2}\rangle - |\overline{2}1\rangle) \\
|v_{-12}^-\rangle \ &= C(|0\overline{1}\rangle - |\overline{1}0\rangle) - (|1\overline{2}\rangle - |\overline{2}1\rangle) \\
\mathfrak{m} = \ \ 0, \mathfrak{p} = \ \ 1, |v_{01}^+\rangle, |v_{02}^+\rangle, |v_{03}^+\rangle : \ &\text{ see below} \\
\mathfrak{p} = -1, |v_{01}^-\rangle \ &= (|1\overline{1}\rangle - |\overline{1}1\rangle) + D(|2\overline{2}\rangle - |\overline{2}2\rangle) \\
|v_{02}^-\rangle \ &= D(|1\overline{1}\rangle - |\overline{1}1\rangle) - (|2\overline{2}\rangle - |\overline{2}2\rangle).
\end{aligned} \tag{3}$$

In this table the canonical spin-2 basis states are denoted as

$$\begin{aligned}
S_i^z|2\rangle = \ \ 2|2\rangle \qquad & S_i^z|1\rangle = \ \ 1|1\rangle \qquad S_i^z|0\rangle = 0 \\
S_i^z|\overline{2}\rangle = -2|\overline{2}\rangle \qquad & S_i^z|\overline{1}\rangle = -1|\overline{1}\rangle \ .
\end{aligned} \tag{4}$$

As can be seen from (3), the local eigenstates are completely fixed in the subspaces $\mathfrak{m} = \pm 4, \pm 3$ and $\mathfrak{m} = \pm 2, \mathfrak{p} = -1$. Except for $\mathfrak{m} = 0, \mathfrak{p} = 1$ the remaining subspaces are two-dimensional. Within such a two-dimensional subspace the eigenstates of h_{ij} can be rotated (but have to be orthogonal), so a *superposition parameter* has to be introduced. In (3) these superposition parameters are denoted as A, B, C, and D.

The subspace $\mathfrak{m} = 0, \mathfrak{p} = 1$ is 3-dimensional, hence a single superposition parameter is not sufficient to cover all possible orientations of the h_{ij} eigenstates within this subspace. Instead, an arbitrary 3-dimensional rotation is necessary to generate the h_{ij} eigenstates from the orthogonal basis

$$|00\rangle,\ |1\overline{1}\rangle + |\overline{1}1\rangle,\ |2\overline{2}\rangle + |\overline{2}2\rangle. \tag{5}$$

This requires 3 continuous parameters. The explicit parametrization within this subspace is not needed in this paper.

Any local interaction operator h_{ij} which obeys symmetries 1 and 2 can be written in terms of projectors onto the local eigenstates (3)

$$h_{ij} = \sum_k \lambda_k |v_k\rangle\langle v_k|. \tag{6}$$

The λ_k are real parameters. Spin-flip invariance (symmetry 3) is achieved by choosing the same λ-coefficients for $S_i^z + S_j^z$ eigenstates corresponding to eigenvalues $\mathfrak{m}$ and $-\mathfrak{m}$. This leads to the following general representation of the local interaction operator:

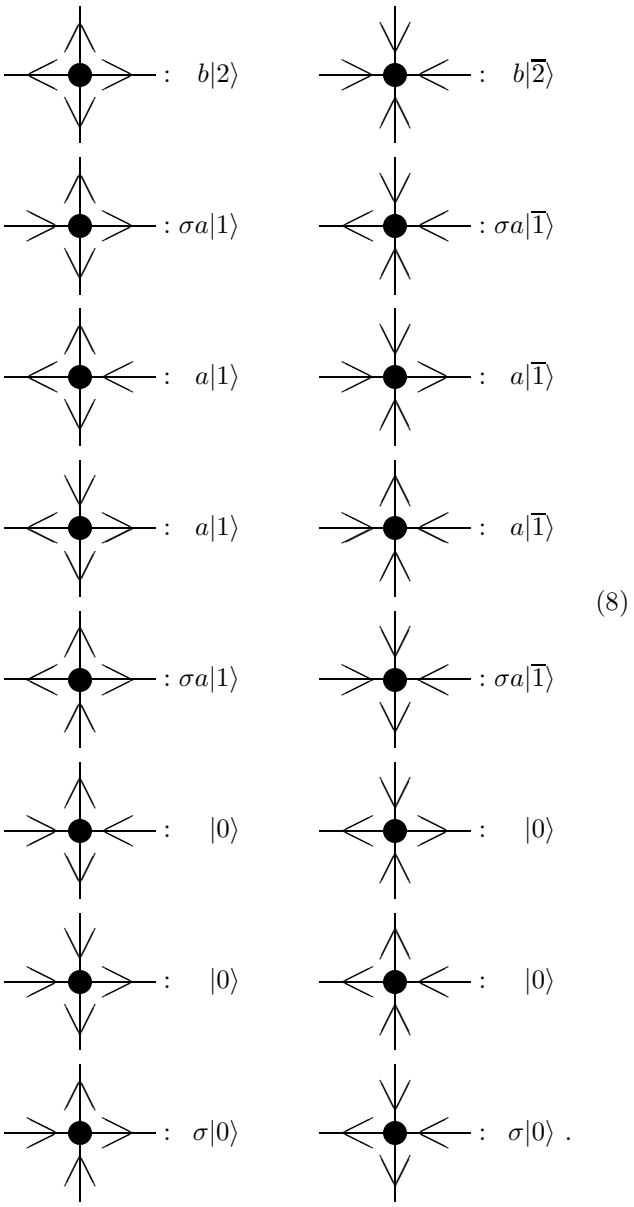
$$\begin{aligned}
h_{ij} \ = \ & \lambda_4(|v_4\rangle\langle v_4| + |v_{-4}\rangle\langle v_{-4}|) \\
& + \lambda_3^+(|v_3^+\rangle\langle v_3^+| + |v_{-3}^+\rangle\langle v_{-3}^+|) \\
& + \lambda_3^-(|v_3^-\rangle\langle v_3^-| + |v_{-3}^-\rangle\langle v_{-3}^-|) \\
& + \lambda_{21}^+(|v_{21}^+\rangle\langle v_{21}^+| + |v_{-21}^+\rangle\langle v_{-21}^+|) \\
& + \lambda_{22}^+(|v_{22}^+\rangle\langle v_{22}^+| + |v_{-22}^+\rangle\langle v_{-22}^+|) \\
& + \lambda_2^-(|v_2^-\rangle\langle v_2^-| + |v_{-2}^-\rangle\langle v_{-2}^-|) \\
& + \lambda_{11}^+(|v_{11}^+\rangle\langle v_{11}^+| + |v_{-11}^+\rangle\langle v_{-11}^+|) \\
& + \lambda_{12}^+(|v_{12}^+\rangle\langle v_{12}^+| + |v_{-12}^+\rangle\langle v_{-12}^+|) \\
& + \lambda_{11}^-(|v_{11}^-\rangle\langle v_{11}^-| + |v_{-11}^-\rangle\langle v_{-11}^-|) \\
& + \lambda_{12}^-(|v_{12}^-\rangle\langle v_{12}^-| + |v_{-12}^-\rangle\langle v_{-12}^-|) \\
& + \lambda_{01}^+|v_{01}^+\rangle\langle v_{01}^+| + \lambda_{02}^+|v_{02}^+\rangle\langle v_{02}^+| + \lambda_{03}^+|v_{03}^+\rangle\langle v_{03}^+| \\
& + \lambda_{01}^-|v_{01}^-\rangle\langle v_{01}^-| + \lambda_{02}^-|v_{02}^-\rangle\langle v_{02}^-|.
\end{aligned} \tag{7}$$

The total number of parameters is 22: there are 15 λ-parameters, the superposition parameters A, B, C, D, and the 3 rotation parameters in the subspace $\mathfrak{m} = 0$, $\mathfrak{p} = 1$. This includes two trivial parameters, namely an offset and a scale.

Equation (7) is the most general interaction operator between adjacent spin-2 sites which has symmetries 1–3. For most values of the 22 parameters the corresponding global Hamiltonian (1) has a very complicated ground state. However, in the next section we shall construct optimum ground states for a submanifold of interaction operators.

3 The vertex state model

Following the procedure explained in [6] we define a set of *vertices* with binary arrow variables on the bonds. On the square lattice there are $2^4 = 16$ different vertices:



(8)

Unlike classical vertices, the "weights" of these vertices are single-spin states $\alpha|\mathfrak{m}\rangle$, where

$$\mathfrak{m} = \frac{1}{2}(\text{number of outgoing arrows} - \text{number of incoming arrows}). \tag{9}$$

The prefactor α is *not* fixed by this scheme. It must be adjusted to satisfy the local ground state condition.

In (8) we have introduced 3 parameters, a and b are real, $\sigma = \pm 1$. Note that b is the coefficient of the $|2\rangle$ and $|\overline{2}\rangle$ states, and the prefactors of the $|1\rangle$ and $|\overline{1}\rangle$ states are either a or σa.

The set of vertices (8) is the two-dimensional analogue to the matrices used in the matrix product technique for spin chains. The global ground state is obtained by attaching a vertex to each lattice site, taking the tensorial product of all generated local spin states, and summing out all bond variables:

$$|\Psi_0\rangle = \sum_{\{\mu\}} \prod_i{}^{\otimes}$$

(10)

A global state of this form is called a *vertex state model*.

The local ground state condition (2) requires that $|\Psi_0\rangle$ is annihilated by every local interaction operator. In case of a vertex state model this is certainly fulfilled if h_{ij} annihilates all two-spin states which are generated by all possible concatenations of neighbouring vertices. The list of all these two-spin states can be easily obtained from the vertices (8):

$$\begin{array}{ll}
|12\rangle + \sigma|21\rangle & |\overline{12}\rangle + \sigma|\overline{21}\rangle \\
a^2|11\rangle + b|02\rangle & a^2|\overline{11}\rangle + b|0\overline{2}\rangle \\
a^2|11\rangle + b|20\rangle & a^2|\overline{11}\rangle + b|\overline{2}0\rangle \\
|01\rangle + \sigma|10\rangle & |0\overline{1}\rangle + \sigma|\overline{1}0\rangle \\
|01\rangle + b|\overline{1}2\rangle & |0\overline{1}\rangle + b|1\overline{2}\rangle \\
|10\rangle + b|2\overline{1}\rangle & |\overline{1}0\rangle + b|\overline{2}1\rangle \\
|00\rangle + \sigma a^2|1\overline{1}\rangle & |00\rangle + \sigma a^2|\overline{1}1\rangle \\
a^2|1\overline{1}\rangle + \sigma b^2|2\overline{2}\rangle & a^2|\overline{1}1\rangle + \sigma b^2|\overline{2}2\rangle .
\end{array} \tag{11}$$

If these 16 pair states are local ground states of h_{ij} then the global state $|\Psi_0\rangle$ is an optimum ground state of H. Comparing (11) with the general form of the eigenstates (3) yields the following conditions for the model parameters:

$$\begin{array}{l}
\lambda_3^\sigma = \lambda_{21}^+ = \lambda_2^- = \lambda_{11}^+ = \lambda_{11}^- = \lambda_{12}^\sigma = 0 \\
\lambda_{01}^+ = \lambda_{01}^- = \lambda_{02}^+ = \lambda_{02}^- = 0 \\
A = \frac{b}{a^2},\ B = C = b,\ D = 0 \\
\lambda_4, \lambda_3^{-\sigma}, \lambda_{22}^+, \lambda_{12}^{-\sigma}, \lambda_{03}^+ > 0 \ .
\end{array} \tag{12}$$

Note that in the 3-dimensional subspace $\mathfrak{m} = 0,\ \mathfrak{p} = 1$, only one two-spin state is not annihilated by the local interaction ($\lambda_{03}^+ > 0$). The corresponding eigenstate is

$$|v_{03}^+\rangle = |00\rangle - \frac{\sigma}{a^2}(|1\overline{1}\rangle + |\overline{1}1\rangle) + \frac{1}{b^2}(|2\overline{2}\rangle + |\overline{2}2\rangle). \tag{13}$$

Conditions (12) reduce the number of free continuous parameters in the Hamiltonian from 22 to 7 (5 λ-parameters and a, b). This includes an overall scale, so the number of non-trivial interaction parameters is 6.

Of course the general local interaction operator (7) can also be written in terms of the canonical single-spin operators S^x, S^y, S^z. In this representation h_{ij} is a polynomial in the three operators $S_i^x S_j^x + S_i^y S_j^y$, $S_i^z S_j^z$, and $(S_i^z)^2 + (S_j^z)^2$, which are all compatible with symmetries 1, 2, and 3. In the present case of spin-2 the polynomial consists of 22 terms. As functions of the parameters introduced above the coefficients of these 22 terms can be obtained by writing the expectation values $\langle v_k|h_{ij}|v_{k'}\rangle$ in

both representations. This yields a set of linear equations for the coefficients.

An important special case with a rather simple Hamiltonian is the *isotropic point*. In this case the ground state parameters are $a = \frac{1}{2}\sqrt{6}, b = -\sqrt{6}, \sigma = -1$, where $|\Psi_0\rangle$ coincides with the VBS ground state on the square lattice discussed in [14]. The corresponding local interaction is the $SO(3)$ invariant operator

$$h_{ij} = \mathbf{S}_i\mathbf{S}_j + \frac{7}{10}(\mathbf{S}_i\mathbf{S}_j)^2 + \frac{7}{45}(\mathbf{S}_i\mathbf{S}_j)^3 + \frac{1}{90}(\mathbf{S}_i\mathbf{S}_j)^4, \quad (14)$$

which projects onto the subspace with maximum total spin $(\mathbf{S}_i + \mathbf{S}_j)^2 = 4(4+1)$. It is shown in [14] that on a finite square lattice with periodic boundary conditions, the VBS state has exponentially decaying two-point correlation functions and no Néel order. In addition, the existence of an energy gap above the ground state is conjectured.

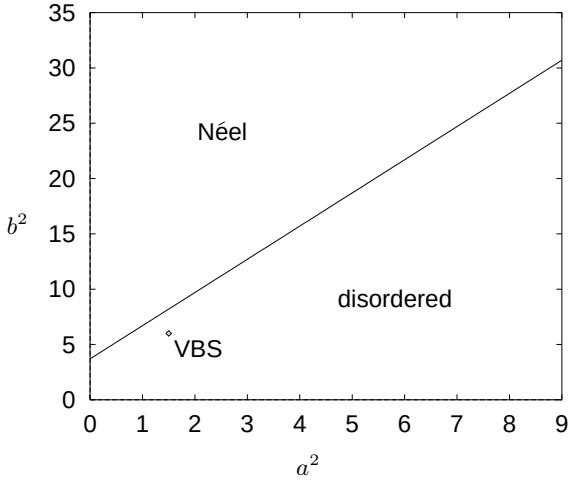


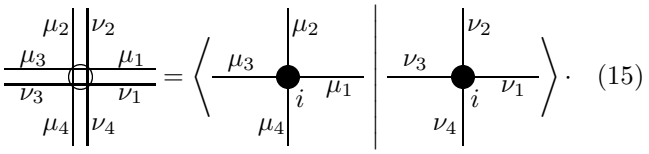
Fig. 1. Phase diagram as a function of a^2 and b^2.

4 Properties of the global ground state

As can be seen from the vertices (8) the constructed ground state $|\Psi_0\rangle$ is invariant under a global spin flip $S^z \to -S^z$ for all values of the parameters a, b, and σ. Therefore the single-spin magnetization and the global magnetization $\langle S^z_{\text{total}}\rangle$ vanish, which indicates an antiferromagnet.

As on the hexagonal lattice there are two noteworthy special cases. In the limit $b \to \infty$ the vertex state model is dominated by the $|2\rangle$- and $|\overline{2}\rangle$-vertices, which can only be arranged in a "checkerboard" configuration. Thus in the limit $b \to \infty$ the ground state is simply the sum of both possible fully polarized Néel states. The other important special case is the *isotropic point*, $a = \frac{1}{2}\sqrt{6}$, $b = -\sqrt{6}$, $\sigma = -1$, which has already been discussed above. Most importantly, it has no Néel order. It will be seen in this section that there are two phases with and without Néel order which are separated by a critical transition line.

In order to calculate properties of the global ground state for general values of the parameters we investigate the inner product $\langle\Psi_0|\Psi_0\rangle$. As explained in [6] it is given by the partition function of the classical vertex model with vertices defined as



(15)

These vertices carry *two* independent sets of bond variables. Their weights are ordinary numbers. Due to the assignment scheme (9) only those classical vertices have a non-vanishing weight, where the number of outgoing arrows on the μ-bonds and on the ν-bonds are equal. Only 70 out of the 256 vertices fulfil this condition. Quantum mechanical expectation values in the vertex state model correspond to statistical expectation values in the classical vertex model (15).

No exact solution of this classical vertex model is available, so we have applied a Monte-Carlo algorithm to this system. As on the hexagonal lattice [6] the model exhibits a phase transition from a disordered phase to a Néel ordered phase. Figure 1 shows the phase diagram, which has been obtained from the numerics.

- For large values of a^2 and small values of b^2 longitudinal correlation functions decay exponentially to zero as a function of distance. There is no long-range order. The global ground state is *disordered*.
- In the opposite case of small a^2 and large b^2, longitudinal correlation functions show an alternating long-range behaviour. The ground state has *Néel order*.

Interestingly, as a function of a^2 and b^2 the phase transition line is a straight line. The slope is 3.0 ± 0.1 and its intercept is given by 3.7 ± 0.3. The analytical explanation of this simple geometrical shape is an open problem.

According to the simulations, the phase transition is of second order. Figure 2 shows the critical correlation function for a system of 30×30 lattice sites at $a^2 = 2$. Agreement with the algebraic function

$$f_l(r) = c_l\left(\frac{1}{\sqrt{r}} + \frac{1}{\sqrt{31-r}}\right) \quad (16)$$

is excellent if c_l is used as a fitting parameter. Therefore, as in the hexagonal lattice case, the critical exponent η is equal to $1/2$.

For the classical vertex model (15) we define $p_{\downarrow\uparrow}$ as the probability to find a pair of antiparallel arrows on a bond. In contrast to the hexagonal lattice $p_{\downarrow\uparrow}$ decays very slowly as a function of the parameters. For instance $p_{\downarrow\uparrow} \approx 3\%$ at $a^2 = 4.0$, $b^2 = 15.7$ (this is in the regime of the phase transition line). Thus vertices with unequal arrow pairs on their bonds (*off-diagonal vertices*) cannot be neglected. Although no reduction to a simpler, exactly solvable model is available, we conjecture that the phase transition corresponds to two simultaneous Ising transitions, as on the hexagonal lattice.

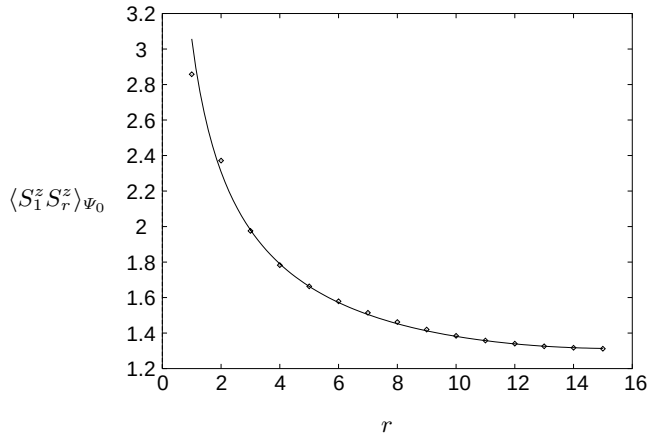


Fig. 2. Critical longitudinal correlation function at $a^2 = 2$ (dots) and the fitted algebraic function (16).

The global ground state is unique for finite system size and $0 < a^2 < \infty, 0 < b^2 < \infty$. The proof is a slightly modified version of the one presented in [6].

5 Conclusion

We have applied the *vertex state model* approach to the ground state problem of a class of spin-2 antiferromagnets on the square lattice. The global ground state contains two continuous parameters a and b which parametrize z-axis anisotropy. Complete $SO(3)$ invariance and extreme Ising anisotropy are contained as special cases.

As the corresponding ground state on the hexagonal lattice, which has been investigated in [6], the system exhibits a second order phase transition from a disordered phase to a Néel ordered phase. For the critical correlation functions we have found $\eta = 1/2$ and conjecture that the transition corresponds to two simultaneous Ising transitions. Interestingly the phase transition line is a straight line as a function of a^2 and b^2.

For the standard spin-2 Heisenberg model on the square lattice with just bilinear exchange the ground state is known to have Néel order. Our results show that this order is destroyed upon introducing higher isotropic spin-exchange operators, however Néel order is restored in the presence of anisotropic terms.

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