Ground state and low-lying excitations of the spin-1/2 $XXZ$ model on the kagomé lattice at magnetization 1/3

A. Honecker$^a$, D.C. Cabra$^b$, M.D. Grynberg$^c$, P.C.W. Holdsworth$^d$, P. Pujol$^d$, J. Richter$^e$, D. Schmalfuß$^e$, J. Schulenburg$^e$

$^a$Technische Universität Braunschweig, Institut für Theoretische Physik, Mendelssohnstrasse 3, 38106 Braunschweig, Germany
$^b$Université Louis Pasteur, Laboratoire de Physique Théorique, 3 Rue de l’Université, 67084 Strasbourg, Cédex, France
$^c$Departamento de Física, Universidad Nacional de La Plata, C.C. 67, (1900) La Plata, Argentina
$^d$Laboratoire de Physique, ENS Lyon, 46 Allée d’Italie, 69364 Lyon Cédex 07, France
$^e$Otto-von-Guericke-Universität Magdeburg, P.O.Box 4120, 39016 Magdeburg, Germany

Abstract

We study the ground state and low-lying excitations of the $S = 1/2$ $XXZ$ antiferromagnet on the kagomé lattice at magnetization one third of the saturation. An exponential number of non-magnetic states is found below a magnetic gap. The non-magnetic excitations also have a gap above the ground state, but it is much smaller than the magnetic gap. This ground state corresponds to an ordered pattern with resonances in one third of the hexagons. The spin-spin correlation function is short ranged, but there is long-range order of valence-bond crystal type.

Key words: Frustration, quantum paramagnet, valence-bond crystal

The spin $S = 1/2$ Heisenberg antiferromagnet on the kagomé lattice has been a focus of intense research during the past decade since it is a hot candidate for an exotic quantum ground state with a frustration-induced spin gap and a continuum of singlet excitations inside this gap (see [1, 2] for recent reviews). Furthermore, a clear plateau at one third of the saturation magnetization ($\langle M \rangle = 1/3$) is found for the $S = 1/2$ $XXZ$ antiferromagnet in the presence of an external magnetic field on the kagomé lattice [3–6]. Here we discuss the nature of the ground state (GS) and low-lying excitations on this plateau.

Fig. 1 shows the spin-spin correlation functions determined numerically for the $S = 1/2$ Heisenberg model on an $N = 36$ kagomé lattice at $\langle M \rangle = 1/3$, i.e. in the GS of the $S^z = 6$ subspace. Note that the finite magnetization gives rise to a constant contribution $1/36 \approx 0.028$ in $\langle S^z_0 S^z_j \rangle$ and $\langle \vec{S}_0 \cdot \vec{S}_j \rangle$. The nearest-neighbor correlations $\langle S^z_0 S^z_1 \rangle \approx -0.0506$ are consistent with an up-up-down spin arrangement around each triangle which would ideally give rise to a value of $-1/12 \approx -0.0833$. Around a hexagon, the sign of the correlations alternates antiferromagnetically from site to site. In particular at larger distances $\langle S^z_0 S^z_j \rangle$ dominates over $\langle S^x_0 S^x_j \rangle = \langle S^y_0 S^y_j \rangle$. Despite the limited distances accessible on the $N = 36$ lattice, it is evident that the spin-spin correlations decay rapidly and are short-ranged.

Further insight can be gained by consideration of the $XXZ$ model [6]. In the Ising limit, the GSs at $\langle M \rangle = 1/3$ are those states where around each triangle two spins point up and one down. These Ising configurations can be explicitly enumerated and the number of configurations $N_{\text{conf}}^I$ determined for a given lattice size $N$ (Table 1 lists a few values). The Ising configurations can be counted asymptotically exactly for large $N$ (see [6, 7] and references therein), and one finds the growth law $N_{\text{conf}}^I \sim (1.1137 \ldots)^N$ on an $N$-site kagomé

To appear in Physica B (proceedings of SCES '04) 14 June 2004
function of the following three-fold degenerate variational lattice, this VBC-type state can be visualized in terms of the Ising model. On the kagomé lattice model on the hexagonal lattice whose GS is a valence-bond crystal (VBC) [8, 9].

The correlations shown in Fig. 1 for the Heisenberg model, defined by half the width of the hexagon $\mathcal{N}^{36}_{\text{eff}}$, are identified by periodic boundary conditions. The radius of the circle at each site $j$ shows the absolute value of the correlation function $\langle \bar{S}_0 \cdot \bar{S}_j \rangle$ for the $S = 1/2$ Heisenberg model at $\langle M \rangle = 1/3$; the big star denotes site 0. Numerical values for all inequivalent correlation functions are shown next to one selected site $j$. The upper number corresponds to $\langle \bar{S}_0^{x} \bar{S}_j^{x} \rangle$, the lower number to $\langle \bar{S}_0^{z} \bar{S}_j^{z} \rangle$.

Finite values of the XXZ anisotropy can be treated within perturbation theory around the Ising limit. The induced transitions between different Ising configurations are described by the effective Hamiltonian [6, 8]

$$\lambda \sum_{\text{hexagon } i} \left\{ \left| \begin{array}{c} 0 \cr 0 \cr 0 \end{array} \right> \langle \begin{array}{c} 0 \cr 0 \cr 0 \end{array} \right| + \left| \begin{array}{c} 0 \cr 0 \cr 0 \end{array} \right> \langle \begin{array}{c} 0 \cr 0 \cr 0 \end{array} \right| \right\} (1)$$

at lowest non-vanishing order and for $N \geq 36$. The sum in (1) runs over all hexagons $i$ of the kagomé lattice. $\lambda > 0$ in the present context.

The effective Hamiltonian (1) is equivalent to a quantum dimer model on the hexagonal lattice whose GS is a valence-bond crystal (VBC) [8, 9]. On the kagomé lattice, this VBC-type state can be visualized in terms of the following three-fold degenerate variational wave function

$$\prod_{\text{hexagon } j} \frac{1}{\sqrt{2}} \left( \left| \begin{array}{c} 0 \cr 0 \cr 0 \end{array} \right> \langle \begin{array}{c} 0 \cr 0 \cr 0 \end{array} \right| - \left| \begin{array}{c} 0 \cr 0 \cr 0 \end{array} \right> \langle \begin{array}{c} 0 \cr 0 \cr 0 \end{array} \right| \right) \prod_{\text{rest } k} \left| t_k \right> (2)$$

where the first product now runs over an ordered $\sqrt{3} \times \sqrt{3}$ pattern of non-overlapping hexagons $j$ (see inset of Fig. 1 of [6]). From (2) one obtains the variational energy $-\lambda N/9$. Although this is only in moderate agreement with the numerically exact GS energies $E^{\text{eff}}_{\text{gs}}$ of (1) for some lattice sizes $N$.

Table 1

| $N$ | $\mathcal{N}^{36}_{\text{eff}}$ | $\mathcal{N}^{36}_{\text{conf}}$ | $E^{\text{eff}}_{\text{gs}}/\lambda$ |
|-----|-----------------|-----------------|-----------------|
| 18  | 13              | 20              | $-4.690415760 \ldots$ |
| 27  | 31              | 42              | $-6.824621992 \ldots$ |
| 36  | 100             | 120             | $-9.970025439 \ldots$ |
| 54  | 884             | 892             | $-13.28992801 \ldots$ |
| 81  | 15 162          | 15 162          | $-17.63317376 \ldots$ |

Table 1

Number of non-magnetic states $\mathcal{N}^{36}_{\text{eff}}$ in the magnetic gap of the Heisenberg model, number of GS configurations $\mathcal{N}^{36}_{\text{conf}}$ of the Ising model, and GS energy $E^{\text{eff}}_{\text{gs}}$ of (1) for some lattice sizes $N$.

To summarize, the $S = 1/2$ Heisenberg antiferromagnet on the kagomé lattice has a three-fold degenerate GS of VBC-type at $\langle M \rangle = 1/3$ and a small gap to all excitations, although there are exponentially many non-magnetic states inside the magnetic gap.

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