SPIN-1/2 HEISENBERG DIAMOND-LIKE DECORATED SQUARE LATTICE IN A MAGNETIC FIELD FROM THE PERSPECTIVE OF LOCALIZED MAGNONS

J. Strečka, jozef.strecka@upjs.sk, K. Karl'ová, katarina.karlova@upjs.sk, Department of Theoretical Physics and Astrophysics, Faculty of Science, P. J. Šafárik University, Park Angelinum 9, 040 01 Košice, Slovakia, A. Honecker, Laboratoire de Physique Théorique et Modélisation, CY Cergy Paris Université, 2 Avenue A. Chauvin, Pontoise, 95302 Cergy-Pontoise, France, andreas.honecker@cyu.fr

ABSTRACT Magnetic and thermodynamic properties of the spin-1/2 quantum Heisenberg model on a diamond-like decorated square lattice are examined using exact numerical diagonalization and an effective description based on a lattice-gas model of hard-core monomers. A hard-core monomer of the effective lattice-gas model corresponds to a localized magnon with a singlet on the decorating bond of the diamond-like decorated square lattice. We show that the effective lattice-gas model provides an accurate description of low-temperature magnetism and thermodynamics in the highly frustrated parameter region $J_2 > 4J_1$. The low-temperature magnetization curve exhibits an intermediate one-fifth magnetization plateau, which persists up to the saturation magnetic field.

INTRODUCTION

Frustrated Heisenberg spin models offer rich magnetic and thermodynamic features [1]. Recently, the ground state of a spin-1/2 Heisenberg model on a diamond-like decorated square lattice has been investigated at zero field [2–4]; the behavior in a magnetic field will be the main subject of the present work.

MODEL

Consider a spin-1/2 Heisenberg model on a diamond-like decorated square lattice (Fig. 1(a)) given by the Hamiltonian:

$$\begin{aligned}\hat{\mathcal{H}} &= J_1 \sum_{i,j} \Big[\hat{\mathbf{S}}_{1,i,j} \cdot \Big(\hat{\mathbf{S}}_{2,i,j} + \hat{\mathbf{S}}_{3,i,j} + \hat{\mathbf{S}}_{4,i,j} + \hat{\mathbf{S}}_{5,i,j} \\ &\quad + \hat{\mathbf{S}}_{2,i-1,j} + \hat{\mathbf{S}}_{3,i-1,j} + \hat{\mathbf{S}}_{4,i,j-1} + \hat{\mathbf{S}}_{5,i,j-1}\Big)\Big] \\ &+ J_2 \sum_{i,j} \Big(\hat{\mathbf{S}}_{2,i,j} \cdot \hat{\mathbf{S}}_{3,i,j} + \hat{\mathbf{S}}_{4,i,j} \cdot \hat{\mathbf{S}}_{5,i,j}\Big) \\ &- h \sum_{i,j} \sum_{k=1}^{5} \hat{S}^z_{k,i,j}, \end{aligned} \tag{1}$$

where $\hat{\mathbf{S}}_{k,i,j} \equiv (\hat{S}^x_{k,i,j}, \hat{S}^y_{k,i,j}, \hat{S}^z_{k,i,j})$ are the spin-1/2 operators assigned to each lattice site and J_1 and J_2 label two nearest-neighbor exchange interactions drawn in Fig. 1(a) by blue and red lines, respectively. Finally, the last term h accounts for the Zeeman coupling of the spin-1/2 particles to an external magnetic field.

The spin-1/2 Heisenberg model on the diamond-like decorated square lattice given by the Hamiltonian (1) exhibits a highly degenerate ground-state subspace in the region $J_2/J_1 > 2$ and at zero field $h = 0$ [2–4]:

$$\begin{aligned}|\{\sigma_{i,j}\}\rangle &= \prod_{i,j} |\sigma_{i,j}\rangle_{1,i,j} \\ &\otimes \frac{1}{\sqrt{2}}(|\uparrow\rangle_{2,i,j}|\downarrow\rangle_{3,i,j} - |\downarrow\rangle_{2,i,j}|\uparrow\rangle_{3,i,j}) \\ &\otimes \frac{1}{\sqrt{2}}(|\uparrow\rangle_{4,i,j}|\downarrow\rangle_{5,i,j} - |\downarrow\rangle_{4,i,j}|\uparrow\rangle_{5,i,j}), \end{aligned} \tag{2}$$

with $\sigma_{i,j} = \uparrow, \downarrow$ corresponding to the z-projections of the nodal spins $S_{1,i,j}$. The states (2) have the character of product states formed by singlets on all decorating bonds and effectively decoupled paramagnetic spins $S_{1,i,j}$ in between. In addition, it can be easily verified that singlets are the lowest-energy flat-band excitations above the fully polarized ferromagnetic ground state in the highly frustrated region $J_2/J_1 > 4$. Hence, it is quite tempting to conjecture that the spin-1/2 Heisenberg model on the diamond-like decorated square lattice is governed by the following effective Hamiltonian in the region $J_2/J_1 > 4$:

$$\mathcal{H}_{\rm eff} = K - h \sum_{i,j} S^z_{1,i,j} - \mu_1 \sum_{i,j} (n_{v,i,j} + n_{h,i,j}). \tag{3}$$

Up to the unimportant constant term $K = N(2J_1 + \frac{1}{2}J_2 - 2h)$ this is equivalent to a set of noninteracting (paramagnetic) spins $S^z_{1,i,j}$ and a lattice gas of hard-core monomers with the chemical potential $\mu_1 = J_2 - h$. The occupation numbers $n_{v,i,j} = 0, 1$ and $n_{h,i,j} = 0, 1$ ascribed to the hard-core monomers determine whether or not a localized magnon (see Ref. [5] for a review), *i.e.*, a singlet is present on a given vertical and horizontal bond, respectively. After straightforward calculation based on the effective Hamiltonian (3) one arrives at the following expression for the free-energy density:

$$\begin{aligned} f &= 2J_1 + \frac{J_2}{2} - 2h - k_{\rm B}T \ln\left[2\cosh\left(\frac{h}{2k_{\rm B}T}\right)\right] \\ &- 2k_{\rm B}T \ln[1 + \exp(\mu_1/k_{\rm B}T)], \end{aligned} \tag{4}$$

where $k_{\rm B}$ is Boltzman's constant and T is absolute temperature. The free energy (4) provides direct access to all magnetic and thermodynamic quantities.

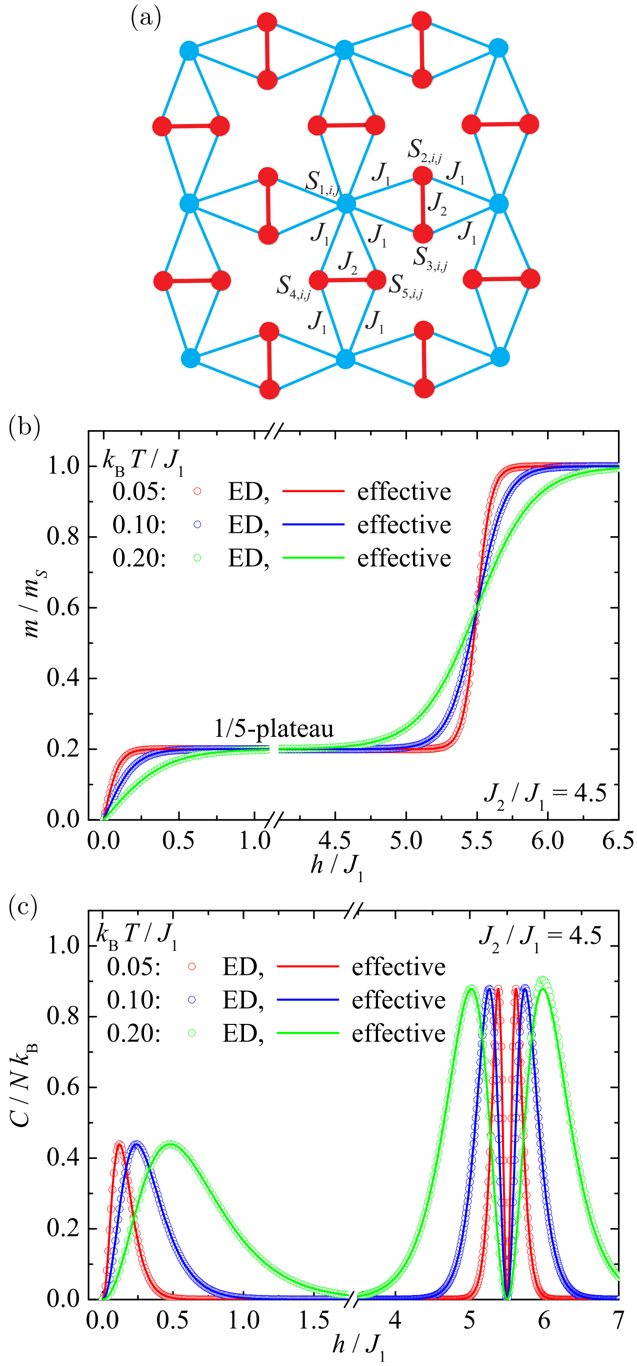

Fig. 1. (a) Part of the diamond-like decorated square lattice. (b) Magnetization curves and (c) specific heat vs. magnetic field for $J_2/J_1 = 4.5$ and three different temperatures. Symbols are ED data for the original model (1) with 5 unit cells (25 spins), solid lines display analytical results for the effective model (3).

RESULTS AND DISCUSSION

Let us confirm validity of the analytical results derived from the effective lattice-gas model (3) by direct comparison with numerical exact diagonalization (ED) of the spin-1/2 Heisenberg diamond-like decorated square lattice (1) subject to periodic boundary conditions. Figs. 1(b,c) demonstrate that isothermal magnetization curves and specific heat obtained from ED and the effective description are in an excellent quantitative agreement up to moderate temperatures $k_{\mathrm{B}}T/J_1 \lesssim 0.2$. The biggest deviation is observed in the specific heat curve for $k_{\mathrm{B}}T/J_1 = 0.2$ around $h = 6J_1$, and may serve as an indication of either deviations from the lattice-gas model or finite-size effects in ED.

The magnetization in Fig. 1(b) exhibits a sudden rise at small magnetic fields to a one-fifth magnetization plateau. This plateau corresponds to the unique state among the set of ground states (2) where all nodal spins $S_{1,i,j}$ are polarized, *i.e.*, all $\sigma_{i,j} = \uparrow$. The one-fifth plateau persists until the saturation magnetic field where the spin dimers are finally also polarized. Just below and above each of these transitions, we find a maximum in the specific heat C shown in Fig. 1(c).

CONCLUSION

In conclusion, we have provided convincing evidence that the effective lattice-gas model of paramagnetic spins and hard-core monomers provides a proper description of magnetic and thermodynamic properties of the spin-1/2 Heisenberg model on a diamond-like decorated square lattice in the highly frustrated parameter region $J_2/J_1 > 4$. A similar effective model has been previously applied to the octahedral chain [6], and it would be interesting to generalize it to other highly frustrated quantum spin models. More concretely, we plan to extend the previous investigations at $h = 0$ [2–4] to the full three-dimensional h-T-J_2/J_1 phase diagram of the spin-1/2 Heisenberg model on the diamond-like decorated square lattice.

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