

Magnetocaloric effect in two-dimensional spin-1/2 antiferromagnets

A. Honecker ^{a,*}, S. Wessel ^b^a *Technische Universität Braunschweig, Institut für Theoretische Physik, Mendelssohnstrasse 3, 38106 Braunschweig, Germany*^b *Universität Stuttgart, Institut für Theoretische Physik III, Pfaffenwaldring 57, 70550 Stuttgart, Germany*

Abstract

The magnetocaloric effect is studied at the transition to saturation in the antiferromagnetic spin-1/2 Heisenberg model on the simplest two-dimensional lattices, namely the square and the triangular lattice. Numerical results are presented for the entropy which are consistent with identical universal properties. However, the absolute values of the entropy are bigger on the geometrically frustrated triangular lattice than on the non-frustrated square lattice, indicating that frustration improves the magnetocaloric properties.

Key words: magnetocaloric effect, quantum phase transitions, frustration*PACS:* 75.30.Sg; 75.10.Jm; 75.50.Ee

Recent theoretical investigations predict an enhanced magnetocaloric effect in geometrically frustrated spin systems at low temperatures [1,2]. Indeed, experiments on the pyrochlore magnet $\text{Gd}_2\text{Ti}_2\text{O}_7$ found substantial drops of temperature around the saturation field during adiabatic demagnetization [3]. These results suggest applications for efficient low-temperature magnetic refrigeration.

Investigations of quantum spin systems on two-dimensional lattices have revealed a plethora of semi-classically ordered and unusual quantum ground states (see [4,5] for recent reviews). Rich behavior is also found in a magnetic field, including plateaux in the zero-temperature magnetization curve and field-induced quantum phase transitions (compare [5,6] and references therein).

However, the magneto-thermodynamics on such lattices has received surprisingly little attention. As a first step we study the quantum phase transition at the saturation field on the square and triangular lattice. The Hamiltonian for a Heisenberg antiferromagnet in an external magnetic field h reads

$$H = J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j - h \sum_i S_i^z. \quad (1)$$

The \mathbf{S}_i are spin $s = 1/2$ operators at site i , $J > 0$ is the exchange constant, and $\langle i, j \rangle$ are nearest neighbor pairs on the given lattice. The magnetocaloric properties are determined by the entropy $S(h, T)$ at temperature T . One approach is to compute $S(h, T)$ from the eigenvalues of the Hamiltonian (1) [2] which are obtained by exact diagonalization (ED) on a finite lattice with N sites. Complete spectra are obtained for $N \leq 21$ while for bigger N we use a truncation procedure valid at low energies [7]. Another approach is to obtain the entropy from a stochastic evaluation of the partition function using an extended ensemble quantum Monte Carlo (QMC) method, based on a flat-histogram formulation [8]. The latter method is restricted to unfrustrated lattices, and we employ it for the square lattice.

Fig. 1 shows the entropy per site S/N as a function of temperature at the saturation field, given by $h_{\text{sat.}} = 4J$ and $9J/2$ for the square and triangular lattice, respectively (see e.g. [6]). This corresponds to a quantum critical point in dimension $d = 2$ with a dynamical critical exponent $z = 2$. According to a scaling theory for the low-temperature physics at such a quantum critical point [9], the entropy should follow a power law

* Corresponding Author. Tel: +49-531-391 5190, fax: +49-531-391 5833

Email address: a.honecker@tu-bs.de (A. Honecker).

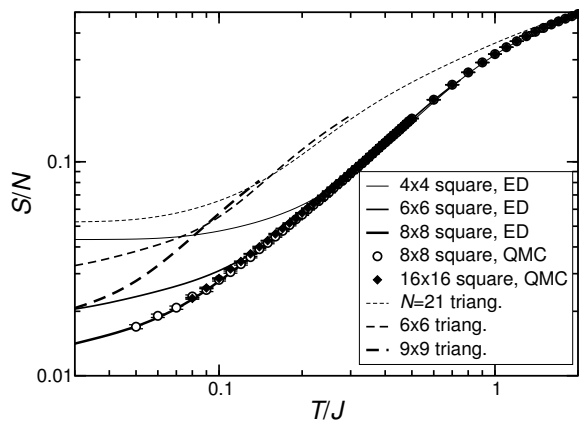


Fig. 1. Entropy per site of the antiferromagnetic $s = 1/2$ Heisenberg model at the saturation field on the square and the triangular (triang.) lattice with N sites as a function of temperature T . Note the doubly logarithmic scale.

$S(h_{\text{sat.}}, T)/N \propto T^{d/z} = T$ with possible logarithmic corrections characteristic for $d = 2$. Finite-size effects are evident at low temperatures in Fig. 1, but at intermediate temperatures the curves collapse onto a line which is consistent with the above universal power law. However, the prefactor is clearly different, *i.e.*, at low temperatures the entropy for the frustrated triangular lattice is roughly twice as big as for the non-frustrated square lattice.

Fig. 2 shows curves of constant entropy in the h - T plane close to the saturation field for (a) the square and (b) the triangular lattice. Since the condition for an adiabatic process is that entropy remains constant, these curves present the behavior of the temperature $T(h)$ during an adiabatic demagnetization process. Finite-size effects are relevant on the 6×6 lattices for $T \lesssim 0.1 J$ (the wiggles at very low T correspond to the different discrete sectors of total S^z at the given system size). Nevertheless, a drop in temperature is evident when the saturation field $h_{\text{sat.}}$ is approached adiabatically from above in both cases. There seems to be a slight heating when the field is further lowered ($h < h_{\text{sat.}}$) for the square lattice (Fig. 2(a)) while temperature stays almost constant on the triangular lattice (Fig. 2(b)). Note furthermore that in the region covered by Fig. 2, the values of the entropy S/N are roughly twice as big on the triangular lattice when compared with the corresponding region of the square lattice, as we have already observed for $h = h_{\text{sat.}}$.

To summarize, the same universal behavior of $S(T)$ is found on the square and the triangular lattice at the saturation field. However, the prefactors are enhanced by frustration, thus improving the magnetocaloric properties of the frustrated triangular lattice as compared to the square lattice, a non-frustrated lattice. Entirely different behavior is expected for highly frus-

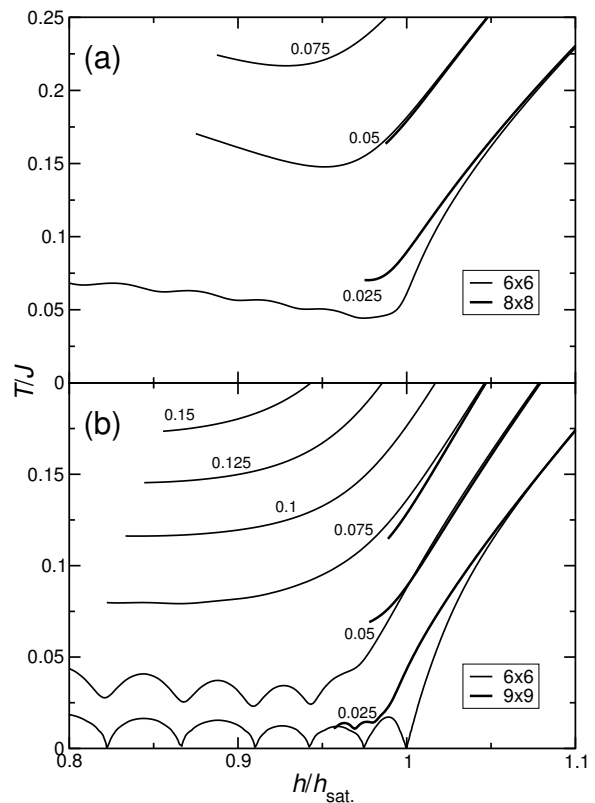


Fig. 2. Curves of constant entropy on the (a) square and (b) triangular lattice in the vicinity of the saturation field $h_{\text{sat.}}$. The values of S/N are indicated by numbers next to the lines.

trated lattices, where at the classical level cooling rates have been found to be up to several orders of magnitude bigger [1]. The magneto-thermodynamics of the corresponding quantum systems remains to be investigated.

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