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Specific heat of the spin-$\frac{1}{2}$ Heisenberg antiferromagnet on *squagome* lattice

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Abstract

The free energy of the spin-$\frac{1}{2}$ Heisenberg antiferromagnet (HAF) on a *squagome* lattice is calculated within the Suzuki–Takano quantum decimation technique. The resulting specific heat exhibits an additional peak in the low-temperature region.

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Two-dimensional quantum Heisenberg spin systems with strong frustration which do not exhibit long-range magnetic order in the ground state are currently a subject of experimental and theoretical interest. There is a lot of numerical evidence suggesting that there exists a gap in the excitation spectrum of such systems. This is an illustration of a general rule which states that if there is a singlet–triplet gap in the excitation spectrum of the Heisenberg system then there is no long-range magnetic order in its ground state [1]. Furthermore, this gap also influences the low-temperature dependence of the specific heat: in the low-temperature region there may exist an additional maximum. According to many numerical studies, see e.g., [2–4], the spin-$\frac{1}{2}$ Heisenberg antiferromagnet on a *kagomé* lattice can serve here as an example.

A *squagome* lattice has been introduced recently. It was suggested [5], using $1/N$ expansion and the mean field approximation, that the Heisenberg antiferromagnet,

$$H = K \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j \qquad (1)$$

on this lattice should have a disordered ground state and two-peak specific heat. $\vec{S}_i$ stands in equation (1) for the spin operator on the site i, K is the positive coupling constant with included temperature and the sum runs over nearest spins. However, the *squagome* lattice is, in fact, the square lattice with additional points put in the middle of edges (decorated), see figure 1. The Heisenberg spins are put on each lattice point and antiferromagnetic interactions are assigned along each edge of the lattice. Clearly, this is not a uniform [6] lattice, i.e. it is not built from regular polygons, such as square, triangular or *kagomé* lattices. Let us stress the fundamental geometrical similarity of the *kagomé* and *squagome* lattices: in both cases the even polygon on the lattice is surrounded only by triangles and vice versa. This similarity

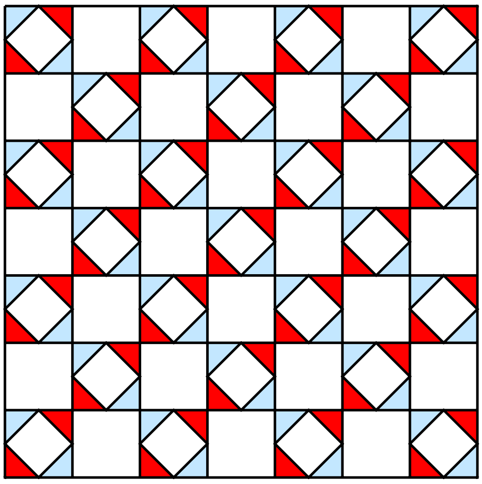

Figure 1. The *squagome* lattice is equivalent to the decorated square lattice with interactions distributed in a 'checkerboard' way. The antiferromagnet on the *squagome* lattice may be formed by putting five-spin clusters (dark and light) from figure 2 together.

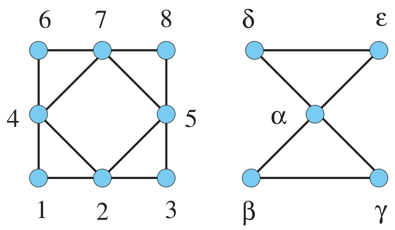

Figure 2. Eight- and five-spin clusters which are the basic blocks for defining the renormalization group transformation.

also manifests in the infinite ground state degeneracy [7] (with respect to rotation of spin vectors) of classical spin systems on both lattices. It was suggested that in the 'quantum' ground state of spin antiferromagnets on such lattices, there can exist independent magnon states [8] and consequently the macroscopic magnetization jumps in the magnetic field [9]. Our main motivation to investigate properties of the Heisenberg model on a *squagome* lattice, being one of 'corner-sharing triangles' lattices, is to show that the origin of low-temperature thermodynamical behaviour is the geometrical structure of these lattices.

In this paper it is reported how one can justify the existence of the low-temperature specific heat peak for the Heisenberg antiferromagnet on the *squagome* lattice within a quantum renormalization scheme proposed by Suzuki and Takano [10, 11]. This method has already been applied to analyse the properties of many spin systems: the one-dimensional Hubbard model [12], a model of a quantum spin glass [13], the $t{-}J$ model [14] and the Heisenberg model on *Sierpiński* fractal and *kagomé* lattices [15, 16]

Let us describe the decimation procedure in more detail. The aim is, as usual, to find a renormalized coupling constant and subsequently to calculate the free energy of the spin system. In the case under consideration it consists of two steps. In the first step, we make a cluster approximation and split the infinite system (Hamiltonian H) into *eight-spin* subsystems (H_i), shown in figure 2. For the *eight-spin* cluster we calculate the partition function $\mathrm{Tr}_{1-8}\exp(-H_i) = Z_i$. Now, recalling that renormalization group transformation should

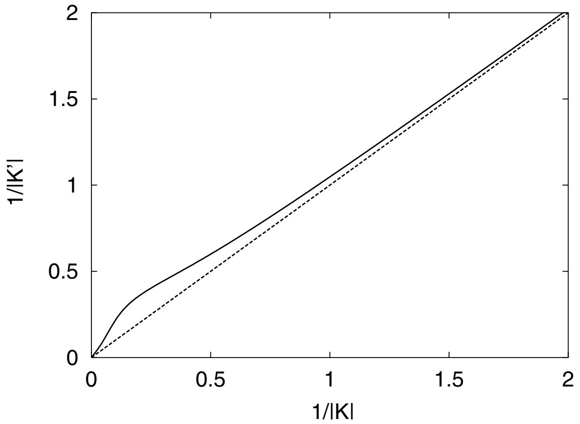

Figure 3. The |renormalized coupling constant|$^{-1}$ versus |coupling constant|$^{-1}$ for the spin-$\frac{1}{2}$ antiferromagnet on a *squagome* lattice.

preserve the partition function we map the Z_i on $Z_i' = \mathrm{Tr}_{\alpha-\epsilon}\exp(-H_i')$ which is the partition function for the cluster of *five* spins $(\alpha \ldots \epsilon)$, shown in figure 2. In the second step, these *five*-spin clusters are put together to obtain the renormalized spin system (Hamiltonian H') on the *squagome* lattice, see figure 1. Five-spin and eight-spin clusters are the smallest systems taking into account frustration. Note that the approximation made here is that we neglect the non-commutativity of the spin operators while splitting the Hamiltonian H into Hamiltonians H_i and subsequently put H_i' together to obtain the renormalized Hamiltonian H', i.e.

$$\exp\left(\sum_i H_i\right) \approx \prod_i \exp(H_i) \approx \prod_i \exp(H_i') \approx \exp\left(\sum_i H_i'\right). \tag{2}$$

Note also that this approximation has been made in opposite directions, and therefore the non-commutative effects have, at least to some extent, been cancelled [10]. The first sum and the first product in equation (2) run over eight-spin clusters, whereas the second product and the second sum run over five-spin clusters on the renormalized lattice. The transformation does not change the partition function, thus

$$\mathrm{Tr}_{1-8}\exp(-KS) = \mathrm{Tr}_{\alpha-\epsilon}\exp(-G - K'S') \tag{3}$$

with

$$S = \vec{S}_1\cdot(\vec{S}_2+\vec{S}_4)+\vec{S}_3\cdot(\vec{S}_2+\vec{S}_5)+\vec{S}_8\cdot(\vec{S}_5+\vec{S}_7) + \vec{S}_6\cdot(\vec{S}_4+\vec{S}_7)+(\vec{S}_2+\vec{S}_7)\cdot(\vec{S}_4+\vec{S}_5) \tag{4}$$

and

$$S' = \vec{S}_\alpha\cdot(\vec{S}_\beta+\vec{S}_\gamma+\vec{S}_\delta+\vec{S}_\epsilon)+\vec{S}_\beta\cdot\vec{S}_\gamma+\vec{S}_\delta\cdot\vec{S}_\epsilon. \tag{5}$$

To calculate effectively the renormalized coupling constant K' one assumes that, as in a case of classical decimation, the correlation function does not change under our renormalization transformation

$$\frac{1}{12}\frac{\mathrm{Tr}_{1-8}[S\exp(-KS)]}{\mathrm{Tr}_{1-8}[\exp(-KS)]} = \frac{1}{6}\frac{\mathrm{Tr}_{\alpha-\epsilon}[S'\exp(-K'S')]}{\mathrm{Tr}_{\alpha-\epsilon}[\exp(-K'S')]}. \tag{6}$$

The renormalized coupling constant is given by the implicit relation (6) and can be calculated numerically. The dependence $K' = \phi(K)$ obtained in this way is shown in figure 3. One

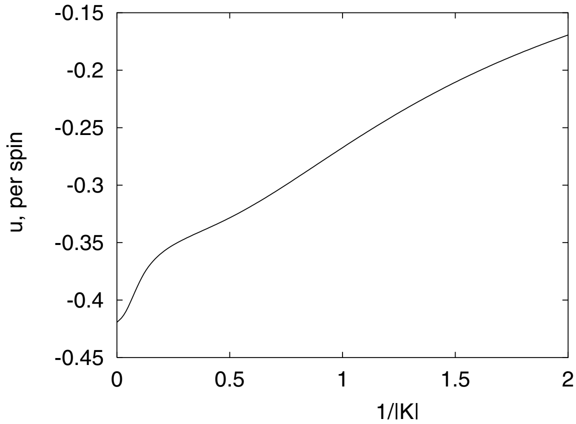

Figure 4. The internal energy (per spin) of the spin-$\frac{1}{2}$ antiferromagnet on a *squagome* lattice.

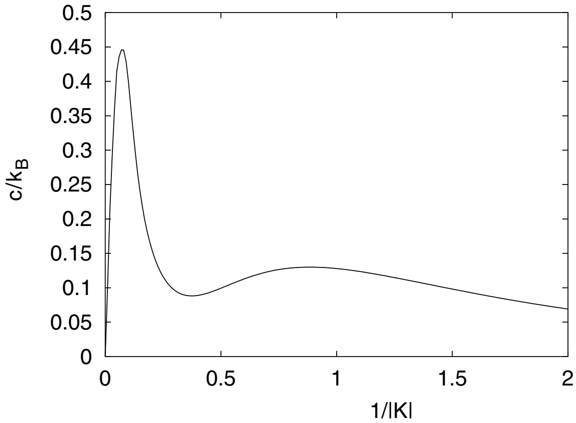

Figure 5. The specific heat (per spin) of the spin-$\frac{1}{2}$ antiferromagnet on a *squagome* lattice.

can see from this figure that RG flow is always towards high temperatures (the dashed line represents the relation $K' = K$). Having obtained the dependence $K' = \phi(K)$ one can calculate from equation (3) the free energy per spin, which transforms as

$$\mathrm{e}^{-Nf(K)} = \mathrm{e}^{-Ng(K)-N'f(K')} \tag{7}$$

with $N = 8$, $N' = 5$ and $G = Ng$. g represents the contribution to the free energy (per spin) from degrees of freedom which have been traced out in RG. Iterating equation (7) one obtains the free energy per spin in the thermodynamical limit

$$-f/k_BT = \sum_{i=0}^{\infty} \left(\frac{5}{8}\right)^i g(K^{(i)}) \tag{8}$$

with $K^{(i)}$ representing the i-times transformed coupling constant K and k_B being the Boltzmann constant. The internal energy of the system under consideration is presented in figure 4. The ground state energy $E_0 = -0.419\,3$ (per spin) while exact diagonalization of finite systems and subsequent extrapolation to the thermodynamic limit gives $E_0 = -0.440\,1$ [7]. In the specific-heat dependence on temperature, which is shown in figure 5, one encounters two peaks. The broad peak located at $T \sim 0.85$ is a typical one whereas the second one, at $T \sim 0.10$, indicates that an additional energy scale is relevant in the system under consideration. A similar feature was observed in a case of frustrated quantum spin systems on other lattices (*kagomé* [4], Δ-chain [17, 18] or *Sierpiński* fractal [15]). The additional energy scale in all those systems seems to be related to the energy of the lowest spin triplet excitation which, although small, does not disappear in the thermodynamic limit. In fact, the energy spectrum of the eight-spin system on a *squagome* lattice (which is Δ-chain, with periodic boundary conditions) with a gap to the triplet excitations is a substantial part of the RG procedure presented here. It was argued [17, 18] that in the case of the Δ-chain, the additional low-temperature peak displayed in the specific heat and reflecting the low-energy part of the energy spectrum is not a 'finite size' effect. Using equation (7) and passing to the thermodynamic limit one meets this gap again in the temperature dependence of the specific heat. This may be a hint that the Heisenberg antiferromagnet on a *squagome* lattice has a disordered ground state. One can also speculate that two-dimensional spin-$\frac{1}{2}$ Heisenberg antiferromagnets containing the Δ-chain-like subsystems will display similar properties.

The total entropy, $\int_0^\infty \frac{c}{T}\,\mathrm{d}T$, corresponding to the calculated dependence c on T is 1.55 ln2 and 80% of this value is related to the first peak. This inconsistency and the difference (4.7%) between the RG ground state energy and its value from exact diagonalization is the result of approximation (2) and the smallness of clusters used in the implementation of the RG procedure. Note, however, that this simple approach seems to capture qualitatively the low-temperature thermodynamics of the Heisenberg antiferromagnet on a *squagome* lattice.

To conclude, we have presented the results of the investigation of the thermodynamical properties of the spin-$\frac{1}{2}$ Heisenberg antiferromagnet on the *squagome* lattice. The temperature dependence of the specific heat strongly suggests that there is no long-range magnetic order in the ground state of this system and there exists a spin gap to the triplet excitations.

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References

[1] Auerbach A 1994 *Interacting Electrons and Quantum Magnetism* (Berlin: Springer) p 67
[2] Lecheminant P, Bernu B, Lhuillier C, Pierre L and Sindzingre P 1997 *Phys. Rev.* B **56** 2521
[3] Waldtmann Ch, Everts H U, Bernu B, Lhuillier C, Sindzingre P, Lecheminant P and Pierre L 1998 *Eur. Phys. J.* B **2** 501
[4] Sindzingre P, Misguich G, Lhuillier C, Bernu B, Pierre L, Waldtmann Ch and Everts H U 2000 *Phys. Rev. Lett.* **84** 2953
[5] Siddharthan R and Georges A 2002 *Phys. Rev.* B **65** 014417
[6] See the collection of uniform lattices at webpage http://www.uwgb.edu/dutchs/symmetry/uniftil.htm
[7] Tomczak P, Schulenburg J, Schmalfuss D and Richter J 2002 Quantum magnetism: microscopic techniques for novel states of matter *288th Heraeus Seminar (Bad Honnef, Germany, 4–6 Nov. 2002)* Abstracts
[8] Schnack J, Schmidt H-J, Richter J and Schulenburg J 2001 *Eur. Phys. J.* B **24** 475
[9] Schulenburg J, Honecker A, Schnack J, Richter J and Schmidt H-J 2002 *Phys. Rev. Lett.* **88** 167207
[10] Suzuki M and Takano H 1979 *Phys. Lett.* A **69** 426
[11] Takano H and Suzuki M 1981 *J. Stat. Phys.* **26** 635
[12] Takano H and Suzuki M 1981 *Physica* A **109** 618
[13] Suan Li Mai and Cieplak Marek 1994 *Physica* A **207** 463
[14] Falicov A and Berker A N 1995 *Phys. Rev.* B **51** 12458
[15] Tomczak P 1996 *Phys. Rev.* B **53** 500R
[16] Tomczak P and Richter J 1996 *Phys. Rev.* B **54** 9004
[17] Kubo K 1993 *Phys. Rev.* B **48** 10552
[18] Nakamura T and Kubo K 1996 *Phys. Rev.* B **53** 6393