Journal of Physics: Condensed Matter

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To cite this article: S S Aplesnin 1998 *J. Phys.: Condens. Matter* **10** 10061

J. Phys.: Condens. Matter **10** (1998) 10061–10065. Printed in the UK PII: S0953-8984(98)90978-X

Quantum Monte Carlo analysis of the 2D Heisenberg antiferromagnet with $S = 1/2$: the influence of exchange anisotropy

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Received 23 January 1998

Abstract. The two-dimensional (2D) Heisenberg model with exchange anisotropy $\Delta = 1 - J^x/J^z$ $(J < 0)$ and $S = 1/2$ is studied by the quantum Monte Carlo method. Energy and spin–spin correlation functions are calculated. The staggered magnetization σ dependence $1/\sigma = 1 + 0.13(1)\ln(1/\Delta)$ on anisotropy exchange is determined.

1. Introduction

In recent times the two-dimensional (2D) quantum spin Heisenberg antiferromagnet (AF) has attracted a great deal of attention in connection with the antiferromagnetic properties of materials with high-temperature superconductivity. Although according to Mermin and Wagner's [1] magnetic theorem the long range order (LRO) at finite temperatures is excluded for the isotropic Heisenberg magnet in 2D, numerous theoretical ground-state (GS) investigations of the 2D Heisenberg AF confirm the existence of LRO at $T = 0$ [2–5]. However, a proof for antiferromagnetic LRO in the GS of the Heisenberg AF is available at present only for $S \geqslant 1$ [6] in the isotropic case or for an anisotropic exchange in the extreme quantum case $S = 1/2$ [7].

Numerical techniques: an exact diagonalization, usually employing Lanczos-like methods [8, 9], and a number of quantum Monte Carlo (MC) methods [5, 10–12] are used for study of the 2D isotropic AF. Exact diagonalization studies are limited to small lattices, since the Hilbert space grows exponentially with the number of sites. MC methods allow us to study very large systems, although application is mostly limited to nonzero temperatures and to study of the isotropic AF. Thus, the nature of the ground state of the 2D antiferromagnet remains unclear. The rather significant quantum fluctuations due to low dimensionality and due to low spin can completely destroy the long range order. Some authors on the basis of analytical methods and the majority of numerical calculations obtain AF order, but others infer the absence of LRO [13, 14].

How can the isotropic 2D Heisenberg model describe the staggered magnetization observed in powder diffraction at low temperatures in La_2CuO_4 [15] and Er_2CuO_4 [16]? The interplanar coupling J' is of the order of 10^{-5} J that is very much less than Ising-like exchange anisotropy $\Delta = 1 - J^x/J^z \sim 10^{-4}$ J [15]. So we need to consider the role of Ising-like anisotropies to study most of the thermodynamic properties of 2D antiferromagnets with CuO_2 planes.

0953-8984/98/4410061+05$19.50

In the paper the quantum Monte Carlo method, using the trajectory algorithm [17] is applied. The algorithm's main idea is based on a transformation of the quantum D-dimensional problem to the classical $D+1$-dimensional one, by using 'temporary ' cuts in the space of imaginary time $0 < \tau < 1//T$ and then realization of an MC procedure in the space 'imaginary time–coordinate' is carried out.

2. Model and method

We shall consider the anisotropic 2D Heisenberg model with negative interactions between nearest neighbours ($J < 0$) on a square lattice with a sites occupied by spins $S = 1/2$, directed along an axis OZ. The Hamiltonian looks like:

$$H = -\frac{1}{2}\sum_{h=1}^{4}\sum_{i=1}^{N}\{J^{zz}(h)S_i^z S_{i+h}^z + J^{x,y}(h)(S_i^x S_{i+h}^x + S_i^y S_{i+h}^y)\}$$

where $\Delta = 1 - J^x/J^z$ is the anisotropy of an 'easy axis' exchange and N is the total number of spins.

The algorithm and MC method have been considered in detail earlier [18, 19]. MC calculations are based on the following Trotter formula [20]:

$$\exp(A_1 + A_2 + A_3 + \cdots + A_p) = \lim_{m\to\infty}[\exp(A_1/m)\exp(A_2/m)\exp(A_3/m)\ldots \times \exp(A_p/m)]^m$$

and the parameter m is called the 'Trotter number'. Hamiltonian is divided into a four spin subsystem

$$H = H_{even}^x + H_{even}^y + H_{odd}^x + H_{odd}^y$$

where $H_{even}^{x,y}$ denotes the sum over four spins on even squares in the x- or y-direction and $H_{odd}^{x,y}$ takes care of the odd squares. We used three kinds of flip into MC procedure. A 'global flip' involves $4m$ spins aligned in the Trotter direction and changes the value of M_z by creating or annihilating a string of down-spins. The deformation and displacement of the strings are taken into account by a 'local flip', which flips two adjacent spins, and also by a 'loop flip', which flips six spins. The MC calculations were performed on the sequence of a lattices linear size of $L = 40$, 48, 64, 80 and $m = 16$, 32, 48 with a periodic boundary condition. For each lattice we used from 1000 to 3000 steps to equilibrate and another from 2000 to 7000 steps to calculate the averages. One MC step is determined by turning all spins on a lattice of dimensions $L \times L \times 4m$.

The following quantities were calculated: the energy, the spin–spin correlation functions of the longitudinal and transverse spin components $\langle S_\alpha(0)S_\alpha(r)\rangle$ along the directions of the lattice sides; the staggered magnetization

$$\sigma = 2\lim_{r\to\infty}\sqrt{\text{abs}\langle S^z(0)S^z(r)\rangle}.$$

The MC method offers three kind of error. The error due to quantum fluctuations yields an estimate $\sim A/(mT)^2$ and for $T/J = 0.1$ it is approximately equal to 2%. The root-mean-square error of the energy is within $\sim$0.1%, the staggered magnetization $\sim$1%.The error due to finite lattice size can be minimized since we made simulations for correlation radius $\xi < L/2$.

3. Results and discussion

The energy and the spin correlation functions of the anisotropic AF at $T \to 0$ we shall determine from the extrapolation of these values estimated for the anisotropic AF at low temperature. We shall calculate temperature dependences of the energy, of the staggered magnetization and of the spin–spin correlation functions for several parameters of anisotropic exchange $\Delta \geqslant 0.005$ and for four lattice sizes and for three m. In extrapolating the data with different Trotter number m, we have used the following $1/m^2$-theorem proved by M Suzuki [20]:

$$C_m = C + a/m^2 + b/m^4 + p/m^6 + \cdots$$

where C_m is the value obtained for the finite decomposition. At every temperature we perform $1/m^2$-extrapolation. The typical dependences are represented in figure 1.

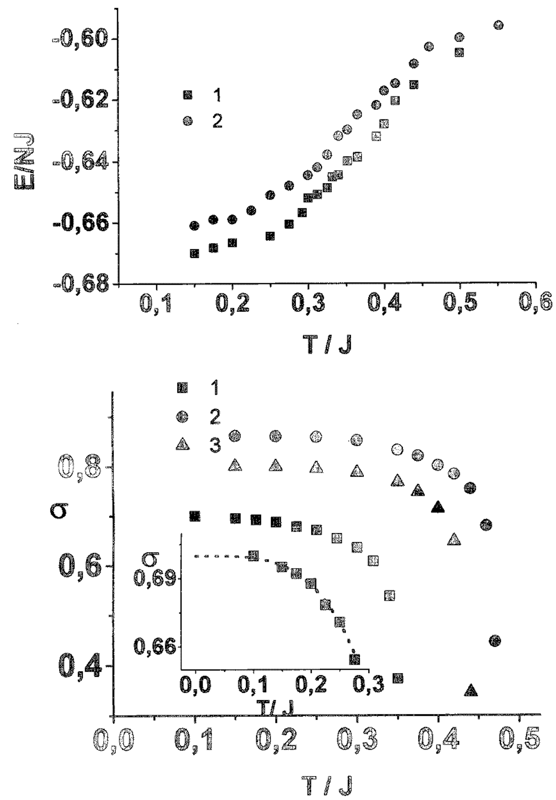

Figure 1. Dependence of the energy E/NJ for exchange anisotropy $\Delta = 0.02(1)$, 0.075(2) and the staggered magnetization of an AF σ for $\Delta = 0.05(1)$, 0.15(3), 0.25(2) on temperature.

In the range of low temperatures, smaller than the energy gap between the GS and excited state $T < 4SJ\sqrt{\Delta(1+\Delta)}$, the calculated value A is interpolated by the power low $A = A(T = 0) - \alpha T^{\beta}$ and the exponential law $A = A(T = 0) - \alpha \exp(-\beta/T)$ (in the inset of figure 1 it is represented by a dotted line) with three fitted parameters α, β and A at $T \to 0$. At these parameters the long spin-wave density is fairly small and they yield an exponentially small contribution to the thermodynamic properties of the 2D

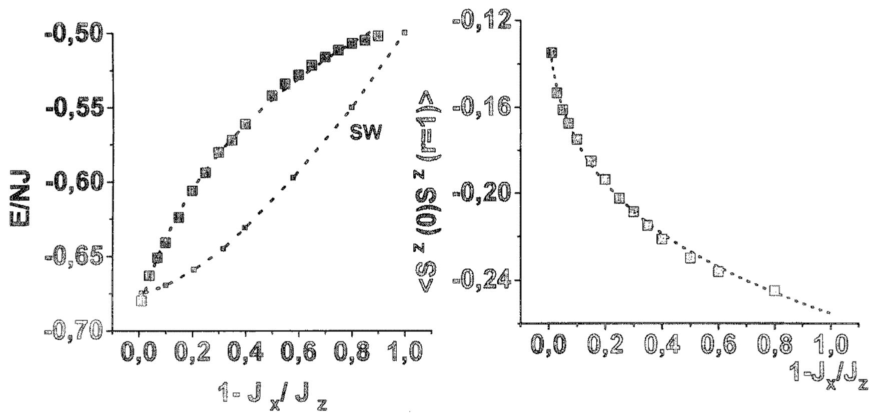

Figure 2. The energy E/NJ and the correlation functions of the nearest neighbour $\langle S^z(0)S^z(r = 1)\rangle$ of an AF at $T \rightarrow 0$ against exchange anisotropy $\Delta = 1 - J^x/J^z$. The curve shown is the estimated second-order spin-wave (SW) prediction [21].

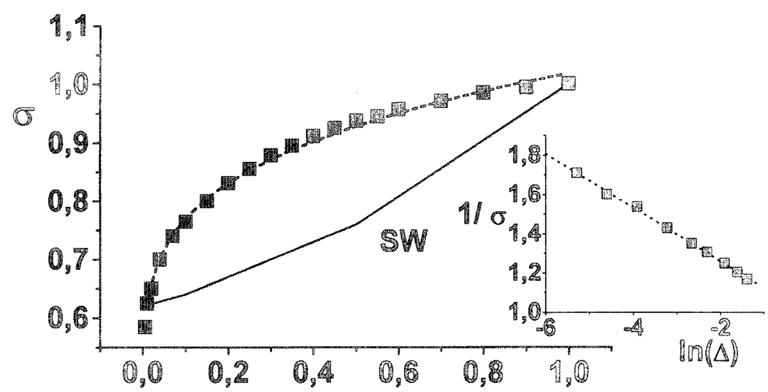

Figure 3. The staggered magnetization (in the inset $1/\sigma$ against $\ln(\Delta)$) of an AF against exchange anisotropy $\Delta = 1 - J^x/J^z$; the curve is SW [21].

antiferromagnet, therefore the quantities of the energy and of the staggered magnetization are practically independent of the lattice size used by the MC procedure. Choice of the interpolation is based on the least value of the root-mean-square EMS δA error.

The extrapolated quantities E and $\langle S^z(0)S^z(r)\rangle$ of the anisotropic AF are represented in figure 2 at $T \rightarrow 0$. They are interpolated by the following function $A = A(\Delta = 0) \pm 1/\exp(\alpha/\Delta^\beta)$ with fitted parameters α, β and $A(0)$. The quantities of parameters are accordingly equal: for the energy $\alpha = 1.61(7)$, $\beta = 0.26(5)$; for the correlation functions $\langle S^z(0)S^z(r)\rangle$ $\alpha = 2.(1)$, $\beta = 0.165(7)$. The energy of the 2D isotropic Heisenberg model $E = -0.684(6)$ at $T \rightarrow 0$ agrees well with the theoretically predicted value by the exact diagonalization method $E = -0.684\,45$ [8]. The spin–spin correlation function $\langle S^z(0)S^z(r)\rangle = -0.120(4)$ is in agreement with the result $\langle S^z(0)S^z(r)\rangle = -0.114$ [3]. In figure 2 our results are compared with spin-wave (SW) analysis (to second order in $1/S$) [21]. The discrepancy may be because of the effect of theoretical correlations in SW are fairly weakly taken into consideration. So the Néel temperature $T_N/J = 0.5$ estimated by the spin-wave theory for the Ising case does not agree with the exact result $T_N/J = 0.564$ [22].

The calculated inverse value of the staggered magnetization fits well to a straight line in the coordinates $1/\sigma - \ln(\Delta)$ shown in the inset of figure 3. The staggered magnetization is interpolated by some functions: the exponential law $\sigma = 1 - A/\exp(B\Delta)$, the polynomial of degree four and the logarithmic law $1/\sigma = 1 + 0.13(1)\ln(1/\Delta)$ (figure 3), which provided the least root-mean-square error. The logarithmic law is based only on numerical grounds and does not appear yet in the literature. The disagreement between the spin-wave data and our results may be due to nonlinear excitation, for example thermally excited skyrmions [23, 24]. The staggered magnetization is $\sigma = 0.58(6)\ \mu_B$ for the value of the exchange anisotropy $\Delta = 0.005$. The calculated values of the staggered magnetization $\sigma = 0.45\ \mu_B$ agree well with experimentally determined values $\sigma = 0.44\ \mu_B$ [15] for La_2CuO_4 with exchange anisotropy $\Delta \sim 10^{-4}$.

So, summarizing, the staggered magnetization of the anisotropic AF depends on exchange anisotropy according to the logarithmic law $1/\sigma = 1 + 0.13(1)\ln(1/\Delta)$ at $T \to 0$.

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