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2000 J. Phys.: Condens. Matter 12 L405

(http://iopscience.iop.org/0953-8984/12/25/104)

J. Phys.: Condens. Matter **12** (2000) L405–L408. Printed in the UK PII: S0953-8984(00)12573-1

LETTER TO THE EDITOR

Quantum renormalization of high-energy excitations in the 2D Heisenberg model

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Received 29 March 2000

Abstract. We find using Monte Carlo simulations of the spin-1/2 2D square lattice nearest neighbour quantum Heisenberg antiferromagnet that the high-energy peak locations at $(\pi, 0)$ and $(\pi/2, \pi/2)$ differ by about 6%, $(\pi/2, \pi/2)$ being the highest. This is a deviation from linear spin wave theory which predicts equal magnon energies at these points.

The simplest model describing quantum antiferromagnets is the nearest neighbour quantum Heisenberg model. Among the class of materials which to a good accuracy can be described by this model are the undoped high-temperature superconductors where the strongly interacting spins are located on a two-dimensional square lattice. Although simple to formulate, the Heisenberg model is not exactly solvable in dimensions greater than one, and approximations or numerical calculations are needed to compare the predictions of the Heisenberg model to experiments.

For the 2D $S = 1/2$ Heisenberg antiferromagnet on a square lattice, the time independent properties are well understood [1–3], and measurements of, for instance, the correlation length [4–7] agree very well with the theoretical predictions. The situation concerning the dynamics is more unclear, and there is a need for definite predictions to which experiments can be compared. In particular, recent neutron scattering measurements on $Cu(DCOO)_2{\cdot}4D_2O$ [8] and La_2CuO_4 [9] directly probe the magnon dispersion between the two points $(\pi/2, \pi/2)$ and $(\pi, 0)$ on the Brillouin zone boundary. These two materials, which are both considered to be physical realizations of the 2D $S = 1/2$ Heisenberg antiferromagnet, show respectively a 6% decrease and a 13% increase in the magnon energy between $(\pi/2, \pi/2)$ and $(\pi,0)$. These results are in contrast to the linear spin-wave approximation of the 2D Heisenberg model, which predicts equal magnon-energies at these points. While these deviations from linear spin-wave theory could be due to additional terms in the Hamiltonian describing each of the materials, it is also possible that there are corrections to linear spin-wave theory. In this Letter we aim at clarifying the predictions for the $S = 1/2$ Heisenberg antiferromagnet on a square lattice at high energies, in particular at the special points $(\pi, 0)$ and $(\pi/2, \pi/2)$ in the Brillouin zone.

The linear spin-wave approximation which is the zeroth term in an expansion in the parameter $1/S$ gives the magnon dispersion

$$\omega_k = 4JS\sqrt{1 - \gamma_k^2} \tag{1}$$

where $\gamma_k = (\cos k_x + \cos k_y)/2$. The wave-numbers are measured in units of the lattice spacing. Note that γ is zero both at $(\pi, 0)$ and $(\pi/2,\pi/2)$.

0953-8984/00/250405+04$30.00

The effect of the first-order correction to linear spin-wave theory is to renormalize uniformly the magnon dispersion by a factor $Z = 1.158$. While there is a question as to what extent one can trust the spin-wave expansion for $S = 1/2$ it has been argued from Monte Carlo measurements [10] that the *only* correction to linear spin-wave theory is such a uniform renormalization of the spectrum. Based on measurements at low energies this renormalization constant is found to be $Z = 1.183$, for $S = 1/2$ [11]. This is similar to the 1D system, where the exact solution gives a uniform renormalization $Z = \pi/2$. In 2D however, there are works which contradict the use of a single uniform renormalization constant. Employing the Dyson–Maleev representation of spin operators, Canali *et al* [12] found that the magnon energy at $(\pi/2, \pi/2)$ is about 2% larger than the magnon energy at $(\pi, 0)$. Expanding around the Ising limit, Singh and Gelfand [13] found a shallow minimum in the dispersion around $(\pi, 0)$ giving the magnon at $(\pi, 0)$ about 7% less energy than at $(\pi/2,\pi/2)$. In addition, an approach to the Heisenberg Hamiltonian starting from the π-flux phase, a state with short-range antiferromagnetic order, predicted a deep local minimum around $(\pi, 0)$ in the Brillouin zone [14].

To clarify this issue we have calculated the dynamic structure factor $S(q, \omega)$ using the quantum Monte Carlo loop algorithm [15], which among other useful features operates in continuous imaginary time [16]. While the simulations are performed in continuous imaginary time, the measurements of the spin–spin correlation function were written to an array with typically 200 points in the imaginary time direction. Typically 10^5 configurations were used both for equilibration and measurements using a single-cluster implementation of the loop algorithm, and all data points are averages of at least five independent runs. The focus on high-energy peaks makes it sufficient to do measurements at intermediate temperatures, $T \sim J$, thus avoiding the low-temperature region where the loop algorithm performs poorly.

To get real-time dynamics from the imaginary time data we employed the maximum entropy method [17], with a flat prior. As we restrict ourselves to only calculating *relative* magnon energies at two points in the Brillouin-zone, this choice of *a priori* information should not be crucial, although we expect that the flat prior overestimates the peak widths. As a check on the continuation procedure we evaluated the sum rules corresponding to the -1, 0 and 1 moments of the dynamic structure function [18]. They were all within the error bars of the quantities, $S(q, \mathrm{i}\omega_n = 0)/2$, $S(q, \tau = 0)$ and $-\epsilon(2 - \cos(q_x) - \cos(q_y))/3$, respectively, which were extracted directly from the imaginary time data (ϵ is the energy per site). A typical picture of the dynamic structure factor thus obtained is shown in figure 1.

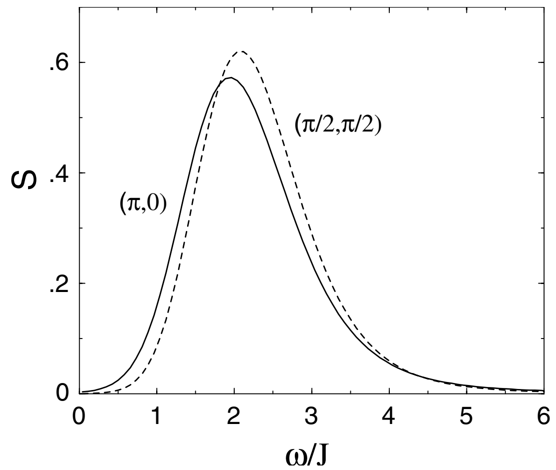

Figure 1. Dynamic structure factor $S(q, \omega)$ at $q = (\pi/2, \pi/2)$ (dashed line) and $q = (\pi, 0)$ (solid line). $T = 0.5J$ and $L = 32$.

Following the approach of Makivic and Jarrell [19], we determined the magnon energy from the normalized first moment ω_q of the relaxation function

$$F(q,\omega) = 2(1 - \mathrm{e}^{-\beta\omega}) S(q,\omega)\,(\beta\omega\chi(q))^{-1}\,. \tag{2}$$

Because there is nothing that breaks the spin rotational symmetry in our Monte Carlo calculation this relaxation function is an average over the transverse and longitudinal relaxation function. This average resembles closely what is measured in neutron scattering experiments.

Computation of ω_q for our smallest systems, 4×4, gives no significant difference between $\omega_{(\pi,0)}$ and $\omega_{(\pi/2,\pi/2)}$. This is in agreement with the exact diagonalization study on small systems of Chen *et al* [10]. However, lattices with 8×8 sites show a clear difference between $\omega_{(\pi,0)}$ and $\omega_{(\pi/2,\pi/2)}$ for all temperatures studied. Performing a finite size analysis for $L\times L$-systems, $L = (4, 8, 16, 32)$, we find that our results are consistent with the finite size behaviour [10] $\omega_{q,L} \approx \omega_{q,\infty} + A_q/L^3$, where A_q is weakly temperature dependent and of order $10J$, and $A_{(\pi/2,\pi/2)} < A_{(\pi,0)}$. The resulting magnon energies for the infinite size system are plotted in figure 2 as functions of temperature.

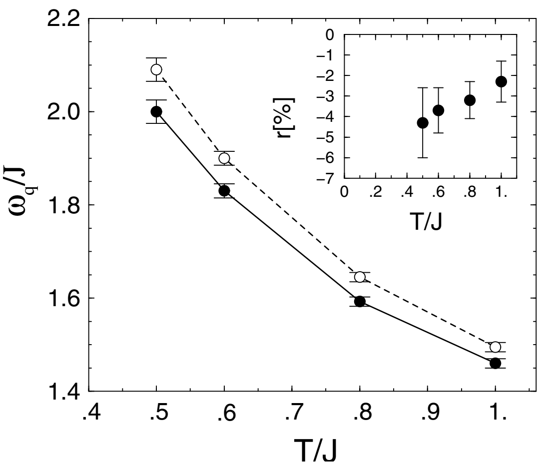

Figure 2. Magnon energies for the two points $(\pi,0)$ (filled circles) and $(\pi/2,\pi/2)$ (open circles) in the Brillouin zone at different temperatures. The inset shows the relative difference $r = (\omega_{(\pi,0)} - \omega_{(\pi/2,\pi/2)})/\omega_{(\pi/2,\pi/2)}$ in percent.

It is clearly seen that the magnon energy at $(\pi,0)$ is *lower* than the magnon energy at $(\pi/2,\pi/2)$. Extrapolating the relative difference to zero temperature we find that the magnon energy at $(\pi,0)$ is about 6% lower than at $(\pi/2,\pi/2)$. This is in rough agreement with the result obtained by expanding around the Ising limit [13].

Comparing this result with the measurements, it is seen that the zone boundary dispersion in $Cu(DCOO)_2\cdot 4D_2O$ is indeed accounted for by the correction to spin-wave theory. Evidence of the zone boundary dispersion has also been observed in $Sr_2Cu_3O_4Cl_2$ which host two interpenetrating square lattices of $S = 1/2$ spins [20]. La_2CuO_4 on the other hand show a significant deviation from our result (19%). This is most likely due to higher-order spin couplings in the Hamiltonian describing this system.

A qualitative explanation for the zone boundary dispersion can be achieved by considering the Hubbard model which for large-U/t at half-filling is equivalent to the Heisenberg model. A reasonable ground state ansatz for the Hubbard model which has a low energy and respects time-reversal invariance is the π-flux state in which the electrons behave as if they were subjected to a magnetic field of flux π per plaquette. In this state the Fermi "surface" is located at the points $(\pi/2,\pm\pi/2)$ in the Brillouin zone, and as the magnons are particle-hole excitations their dispersion will have minima at $(0,\pi)$ and $(\pi,0)$ as well as at $(0,0)$ and (π,π). This qualitatively explains the zone boundary dispersion, but implies at the quantitative level gapless magnons at (π,0) and (0,π). However, the π-flux phase has no antiferromagnetic long-range order, and so it is necessary to do a more refined ground state ansatz to get a quantitative explanation. By considering a ground state consisting of both a π-flux state and a spin density wave (SDW) state which does have a staggered magnetic moment, Hsu [14] found using a Gutzwiller projection technique that the total energy of this combined state could be decreased from the pure π-flux state. Using the random phase approximation he found a shallower zone boundary minimum than for the pure π-flux state. Though still much deeper than what is observed in the present study, the depth of the zone boundary dispersion at (π,0) depends crucially on how much of the ground state is an SDW, as a pure SDW state gives a dispersion identical to linear spin wave theory [21]. It is at present unclear whether a more refined analysis would lead to a better quantitative agreement with our result, but we feel that attributing the zone boundary dispersion to properties of the π-flux state is a plausible, simple and attractive scenario.

Until now, there has been an unsatisfactory situation, where different approximative analytical approaches disagreed on the existence of a zone boundary dispersion in the 2D $S = 1/2$ Heisenberg antiferromagnet on a square lattice. Recent experiments on physical realizations of the model system have strengthened the need to resolve this question. By performing finite temperature quantum Monte Carlo simulations, we have established that indeed there is a zone boundary dispersion. In a system, which is otherwise well described by a uniform renormalization of linear spin-wave theory, the zone boundary dispersion is a remarkable quantum effect.

We would like to thank Patrick Lee, Radu Coldea *et al* and Rajiv R P Singh for useful discussions, and acknowledge the use of the supercomputing facilities at UNI-C, Aarhus University.

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