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LETTER TO THE EDITOR

Quantum Monte Carlo study of a two-dimensional Heisenberg antiferromagnet with non-magnetic impurities

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Abstract. The magnetic properties of a two-dimensional spin-$\frac{1}{2}$ Heisenberg antiferromagnet with non-magnetic impurities is studied by the quantum Monte Carlo method. The combined effect of quantum effects and dilution on the ordering process is investigated. In particular, the dependence of sublattice magnetization on impurity concentration is calculated. It is found that the staggered order has its maximum value at a finite concentration of non-magnetic impurities (~13%) but not at the pure system.

Spin-$\frac{1}{2}$ magnetic insulators have attracted renewed interest in connection with high-T_c superconducting materials. Several experimental investigations of the magnetic properties of the oxide superconductors $La_{2-\delta}Sr_\delta CuO_4$ [1] and $Y_1Ba_2Cu_3O_{6+\delta}$ [2, 3] have stimulated this activity.

In this letter we report first results of a quantum Monte Carlo (QMC) calculation of the magnetic properties of the $d = 2$ Heisenberg antiferomagnet with non-magnetic impurities. Whereas theoretical efforts to understand the systems of interest usually concentrate on the Hubbard model (see e.g. [4-6]), the Heisenberg model (i.e. the large-U limit of the Hubbard model for half-band filling) with immobile impurities is technically much simpler (avoiding 'the minus-sign problem' for the fermions in QMC) and enables us to deal with larger lattices. The model is both of primary theoretical interest, namely the effect of dilution for systems with strong quantum fluctuations, and has significance for actual experiments. Our results are probably most relevant for substances like $Nd_{2-\delta}Ce_\delta CuO_4$ [7], where doping creates magnetic dilution rather than frustration.

The model is described by the following Hamiltonian:

$$H = 2 \sum_{\langle i,j \rangle} \boldsymbol{S}_i \boldsymbol{S}_j \tag{1}$$

where S_i are spin operators ($S_i = \frac{1}{2}\sigma_i$) and i and j are nearest neighbours on a square lattice. For the pure model, QMC calculations have shown that the system has a strongly correlated ground state [8, 9] and have strongly suggested the existence of an ordered ground state [8], in agreement with spin-wave calculations [10, 11]. At finite temperatures the system is disordered with, however, a correlation length diverging as

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$\exp(a/T)$ [12, 13]. By holes we mean missing spins; this is equivalent to all coupling strengths between the hole and the surrounding spins being zero. These holes are static and cannot move through the lattice. This approach is related to the work of Morgenstern [14] but is different in detail; his work concentrated on the effect of frustrated bindings. Since the order in the ground state results from a subtle competition between cooperative interactions and quantum fluctuations, the influence of impurities is of particular interest. In classical systems, an increasing concentration of impurities clearly weakens cooperative interactions and thus finally destroys order even in the ground state, but in systems with strong quantum fluctuations the effect of dilution is not obvious. In this letter, we report some evidence which shows the failure of the simple classical scenario. In particular, we find that the Néel order is enhanced at some finite impurity concentration. This may suggest that a small amount of impurities weakens quantum fluctuations and supports the tendency to classical order.

We study the system by the quantum Monte Carlo method, as formulated by Suzuki [15]. We study systems on the square lattice with $L * L$ sites up to $L = 16$ and Trotter number $n = 48$ for hole concentrations δ less than 50%. The method for the present model has been described in detail in the previous work of one of the authors [9] for the pure case. Here we extend this method in order to include impurities, which requires larger matrix dimensions for the Boltzmann factor of the unit cell (3^8 instead of 2^8 as previously used). Details of the method will be reported elsewhere [16]. Periodic boundary conditions are applied in all directions. We calculate the energy, the squared staggered magr etization (which is used as the order parameter)

$$\langle N_z^2 \rangle = \left\langle \left(\sum_{i \in A} \sigma^z - \sum_{i \in B} \sigma^z \right)^2 \right\rangle \tag{2}$$

where A and B denote the two sublattices, and the staggered susceptibility as discussed in [9]. We have included global flips in x, y and in the Trotter direction which mean that a line of spins may be flipped at the same time, changing particle- and winding-number, respectively [17]. The ergodicity and convergence are tested by comparison with exact calculation in the $L = 4$ systems, using the matrix iteration method. These results agree well with the QMC data for $T = 0.2$. The ergodicity problem in diluted systems is much more complicated than for the pure case. But, a comparison of data and without global flips in x and y directions shows no significant difference if the iteration is sufficiently long. Hole positions are chosen at random for each sublattice separately. Thus systems are specified by numbers of impurities on A and B sublattices, N_A and N_B, respectively. The δ is defined as $\delta = (N_A + N_B)/N$. The ratio of N_A to N_B is important when we study the magnetic susceptibility. If we choose different hole numbers for each sublattice the magnetization of the ground state is not necessarily zero (see also reference [16]). So far we have not performed averaging over samples with different hole positions, partly because we are currently interested in individual phenomena in diluted systems and also because it is too time consuming. Of course, averaging has to be performed to obtain physical quantities in diluted systems. Tests for some concentrations show no difference in the qualitative behaviour.

The convergence for the large systems at low temperatures is very slow and takes up to 350 000 MCS. The deviation due to the Trotter decomposition is of the order $1/n^2$ so we run the simulation for several n-values and fit the data to a polynomial in $1/n^2$ by a least-squares fit. The error in the extrapolation $n \to \infty$ is smallest for a quadratic fit and less than 4%. Comparison with a cubic fit, namely up to $1/n^6$, shows no significant difference and could be used as a test for convergence.

The data for $T = 0.2$ in units of the exchange energy seem to represent the ground state reasonably well, in particular for the lower hole concentrations. The total energy shows an increase with hole concentration δ (figure 1) as expected. The data points for each lattice size nearly lie on one linear curve. The order parameter shows much more interesting behaviour. The square of the total sublattice magnetization $\langle N_z^2/L^4 \rangle$ (i.e. the value per site, not per spin) has a maximum at non-zero hole concentration for system sizes greater than $L = 4$, and vanishes near $\delta \approx 40\%$ (figure 2). This agrees with the site percolation threshold $\delta = 0.41$ [18]. Systems with L greater than 6 show the maximum value at $\delta \approx 13\%$, that is they show a non-monotonic dependence on the concentration. This unexpected behaviour seems to be reinforced with increasing system size. The same behaviour is seen in other systems with different hole positions. This non-monotonicity is also found in the staggered suceptibility. The data for $\delta = 0$ agree with those of [8, 9] (a factor of 4 comes from the different normalization in the former).

The temperature dependence of the sublattice magnetization for $L = 12$ and for different concentrations is plotted in figure (3). Here we see that the non-monotonicity is a phenomenon at low temperature, which strongly suggests that it is largely due to quantum effects. For higher temperatures the lines cross and $\delta = 0$ becomes the highest value. The behaviour at lower temperatures will be documented in a further report. In figure (4) the temperature dependences for $\delta = 12.5\%$ are shown for various system sizes. The decrease of the sublattice magnetization in T is faster for larger systems than for smaller ones. This can be explained with reference to the finite correlation length.

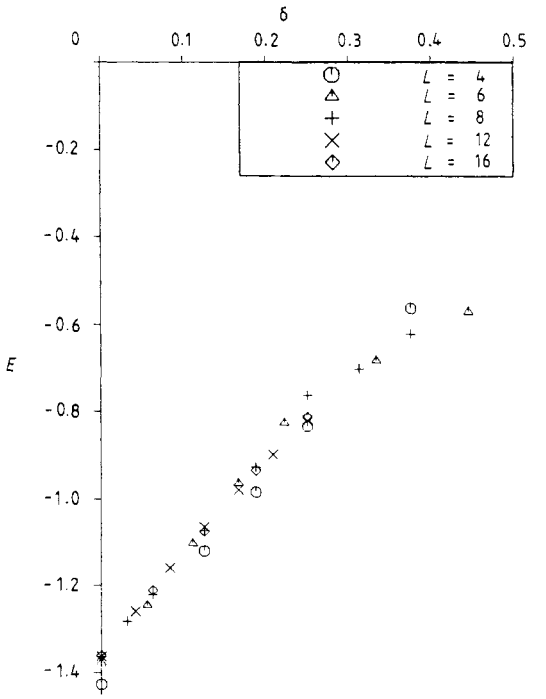

Figure 1. Energy against hole concentration for different system sizes ($T = 0.2$).

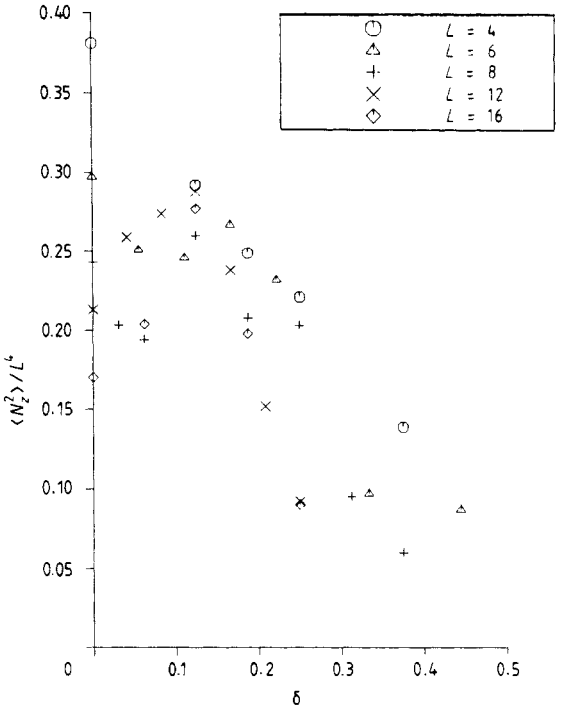

Figure 2. Sublattice magnetization against hole concentration for different system sizes ($T = 0.2$).

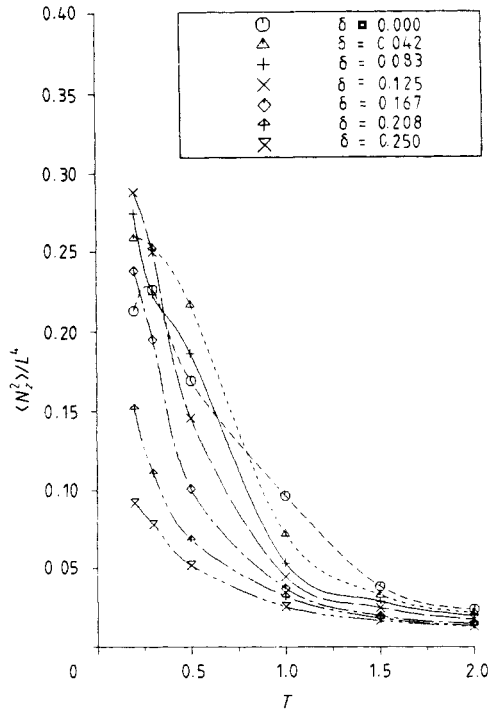

Figure 3. Sublattice magnetization against temperature for $L = 12$. (Lines are drawn to guide the eye. Concentration for each symbol is given in the inset.)

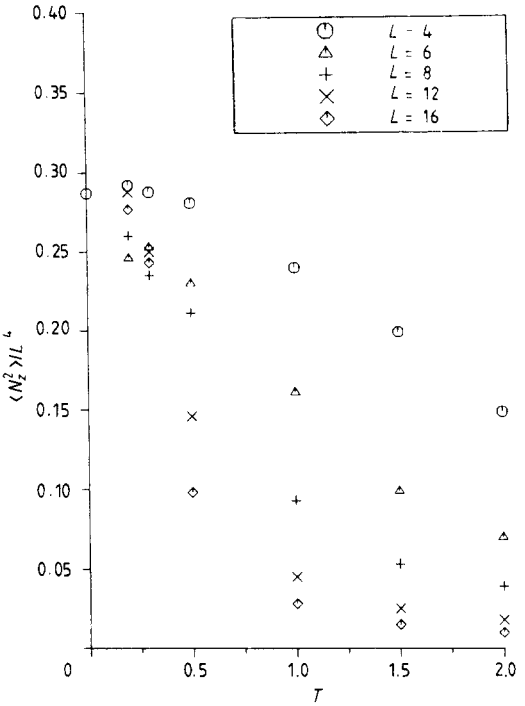

Figure 4. Sublattice magnetization against temperature for different system sizes and $\delta = 12.5\%$. (Lines are drawn to guide the eye. System size for each symbol is given in the inset.)

Our results show that the effect of holes in the $S = \frac{1}{2}$, $d = 2$ Heisenberg antiferromagnet is to suppress quantum fluctuations. For small hole concentrations the ground state becomes closer to the classical Néel state and the sublattice magnetization increases, while for larger hole concentrations the vanishing of long-range order is determined by the percolation threshold (as in the classical model). At present we have no explanation, from first principles, for this observation at low concentrations which contradicts naive expectations and may be the result of a subtle combination of quantum effects, finite-size effects and finite temperatures. The mechanism of this non-monotonicity should contribute to the understanding of quantum fluctuation and should be clarified in the future. This unexpected behaviour of the impure system is not obtained when the effect of impurities is taken into account via the change in the spin-wave spectrum as calculated recently [19]. The decrease in spin-wave energy with δ implies a corresponding decrease in the order parameter. The effect of the impurities as observed in our calculations thus appears to be strongly localized and clearly calls for further theoretical and experimental investigations.

We have also found similar non-monotonic behaviour in the staggered susceptibility and magnetic susceptibility. This will be reported elsewhere.

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