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LETTER TO THE EDITOR

The pair correlation function in the ground state of the two-dimensional spin-$\frac{1}{2}$ XY model

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Abstract. The decay to a constant value of the correlation function $\langle S_0^x S_r^x \rangle$, in the ground state of the spin-$\frac{1}{2}$ XY ferromagnet in two dimensions, is found to be exponential.

In this Letter we examine the ground-state pair correlation function of the two-dimensional spin-$\frac{1}{2}$ XY model. The Hamiltonian for this model is

$$\mathcal{H} = -2J \sum_{\langle ij \rangle} (S_i^x S_j^x + S_i^y S_j^y) \tag{1}$$

where the S_i are the usual quantum mechanical spin operators and the sum is over nearest-neighbour pairs.

Mermin and Wagner (1966) proved that this model has no long-range order for $T > 0$. Nevertheless, it is generally believed that this model undergoes a phase transition at a finite temperature associated with the unbinding of vortex pairs (Kosterlitz and Thouless 1973). Above the transition temperature the spin–spin correlations $\langle S_0^x S_r^x \rangle$ decay exponentially. Below the transition, in the topologically ordered phase, these correlations decay as a power of the separation distance r. This behaviour is usually expressed in terms of the exponent η:

$$\begin{aligned} \langle S_0^x S_r^x \rangle &\propto 1/r^{d-2+\eta} \\ &= 1/r^{\eta}, \qquad d = 2. \end{aligned} \tag{2}$$

In the classical or $s = \infty$ case the Kosterlitz–Thouless theory implies that $\eta = \frac{1}{4}$ at T_c. Spin-wave (Wegner 1967), and renormalisation-group (Amit *et al* 1980) calculations indicate that η is proportional to T as T approaches zero. At $T = 0$, however, there appears to be a first-order transition into a state with non-zero long-range order. In fact, by extrapolating to the thermodynamic limit from finite-lattice calculations, Oitmaa and Betts (1978) estimate

$$\begin{aligned} \langle M_x^2 \rangle / N^2 = N^{-1} \sum_r \langle S_0^x S_r^x \rangle &= 0.116 \pm 0.0002 \text{ (square)} \\ &= 0.104 \pm 0.002 \text{ (hexagonal)} \end{aligned} \tag{3}$$

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for the ground state of the spin-$\frac{1}{2}$ XY model. Here N is the number of sites in the finite lattice. The expression (2) is therefore inappropriate in this case. Jullien *et al* (1980) have apparently overlooked this and calculated a ground-state value of $\eta = 1.21$ for a ferromagnetic spin-$\frac{1}{2}$ XY model on a triangular lattice.

There are two possibilities. Either

$$\langle S_0^x S_r^x \rangle \sim \langle S_0^x S_\infty^x \rangle + A/r^a \tag{4}$$

or

$$\langle S_0^x S_r^x \rangle \sim \langle S_0^x S_\infty^x \rangle + B\mathrm{e}^{-br} \tag{5}$$

as $r \to \infty$.

We have analysed the data from finite-cell calculations on the square and hexagonal lattices to determine which of these two possibilities obtains. Most of these data were available from the work of Oitmaa and Betts; however, the 20-site cell on the square lattice was a new calculation requiring the construction of a matrix of dimension 2403 and determination of its dominant eigenvalue and corresponding eigenvector.

The relatively small size of the finite cells permits evaluation of pair correlations for only a limited separation r. Discriminating between (4) and (5) is therefore not a simple matter. It has proved useful to compute the moments

$$\mu_m(N) = N^{-1} \sum_r (\langle S_r^x S_0^x \rangle_N - \langle S_0^x S_\infty^x \rangle) r^m \tag{6}$$

for several values of m. As N gets large these sums will approach zero or diverge depending on whether m is less than or greater than the leading power in (4). We have computed these moments for $N = 8, 10, 16, 18$ and 20 on the square lattice, and $N = 6, 8, 14$ and 18 on the hexagonal lattice. The results are shown in figures 1 and 2. In both

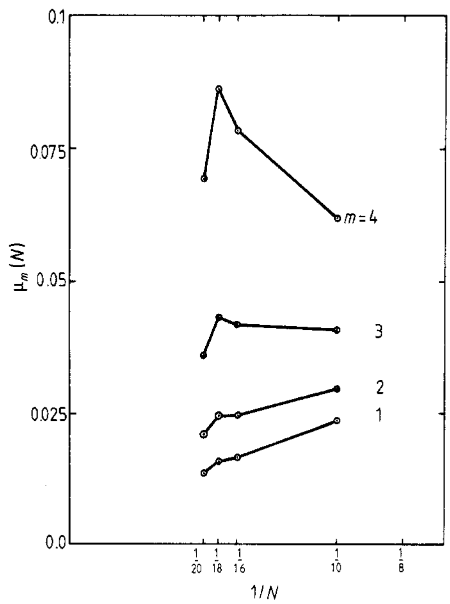

Figure 1. Plot of the moments $\mu_m(N)$ for several values of m on the square lattice.

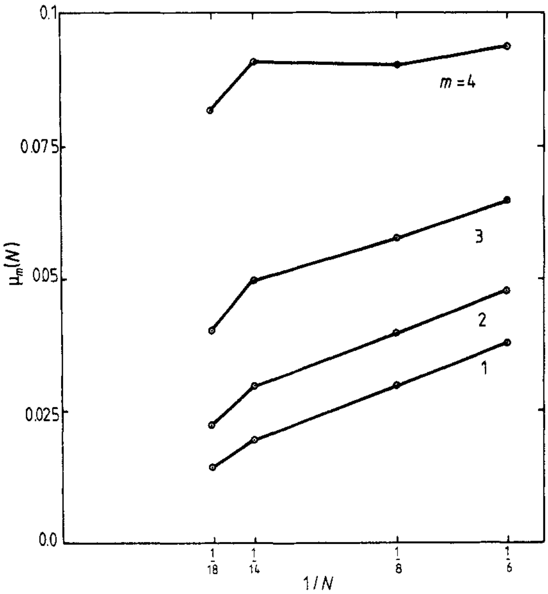

Figure 2. Plot of the moments $\mu_m(N)$ for several values of m on the hexagonal lattice.

cases, for values of m as large as four, the final tendency of the sums is towards zero. From this we conclude that the pair correlations approach a constant value exponentially fast.

The value of b in equation (5) can be estimated from the semi-log plot in figure 3. This gives a value of $b \simeq 1$ for both the square and hexagonal lattices.

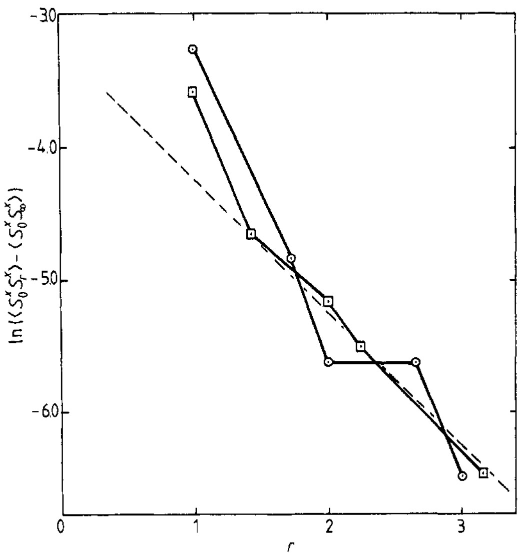

Figure 3. Plot of ln $(\langle S_0^x S_r^x \rangle_N - \langle S_0^x S_\infty^x \rangle)$ against r for $N = 20$ on the square lattice (squares) and $N = 18$ on the hexagonal lattice (circles). The broken line has a slope of -1.

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