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1989 J. Phys.: Condens. Matter 1 1855

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Monte Carlo simulations of the spin- $\frac{1}{2}$ Heisenberg antiferromagnet in two dimensions

J D Reger[†], J A Riera and A P Young

Physics Department, University of California, Santa Cruz, CA 95064, USA

Received 1 August 1988

Abstract. We describe the results of Monte Carlo simulations of the spin- $\frac{1}{2}$ Heisenberg antiferromagnet on the honeycomb lattice. We find that the staggered magnetisation is non-zero and given, quite accurately, by spin-wave theory. Similar results have been found earlier for the square lattice.

1. Introduction

The relevant role that the Cu–O planes play in the recently discovered high- T_c superconductors (Bednorz and Müller 1986, Wu *et al* 1987) and the assumption that the pairing mechanism is associated with antiferromagnetic spin fluctuations (Anderson 1987, Baskaran *et al* 1987, Emery 1987, Hirsch 1987, Ruckenstein *et al* 1987) have raised interest in Hubbard and extended Hubbard models in two dimensions. In particular, the antiferromagnetic spin- $\frac{1}{2}$ Heisenberg model on a square lattice, which corresponds to the half-filled band limit of the Hubbard model, should give a good description of the magnetic properties of the related non-doped insulating materials, such as La_2CuO_4 (Shirane *et al* 1987). With this motivation, there has been recently an extensive study of the ground state of the antiferromagnetic Heisenberg model on two-dimensional lattices. As it is well known, the value of the ground-state staggered magnetisation, m^\dagger , is reduced from its Néel, or classical, value due to quantum mechanical fluctuations. In the spin-wave approximation (Anderson 1952, Kubo 1952, Oguchi 1960), this zero-point deviation is finite for any two-dimensional lattice, implying that a long-range order survives. On the other hand, Anderson (1987) has suggested that high- T_c superconductors may be realisations of the resonant valence bond (RVB) state, originally proposed as the ground state of the spin- $\frac{1}{2}$ Heisenberg antiferromagnet on the triangular lattice. This has led to speculations that the ground state of this model on the *square* lattice may be an RVB state, in which case spin-wave theory would be qualitatively wrong in predicting a finite staggered magnetisation.

Spin-wave theory is the first term in an expansion in powers of $1/(zS)$, where S is the spin and z the coordination number, which is not small for spin- $\frac{1}{2}$ systems on two-dimensional lattices. It is therefore of interest to study the spin- $\frac{1}{2}$ antiferromagnet on two-dimensional lattices by other techniques. Recent studies for the square lattice using

[†] Present address: Institut für Physik, Johannes-Gutenberg-Universität, Postfach 3980, D-6500 Mainz, Federal Republic of Germany.

quantum Monte Carlo simulations (Reger and Young 1988, hereafter referred to as RY, Gross *et al* 1988), diagonalisation of small systems (Tang and Hirsch 1988), and a reanalysis of a perturbation series (Huse 1988) all concur that there *is* long-range order and that the value of the staggered magnetisation is given fairly accurately by spin-wave theory. In addition, Kennedy *et al* (1988) have derived rigorous bounds which are not quite tight enough to prove long-range order in two dimensions for spin- $\frac{1}{2}$, though they do prove this for spin-1 and for a spin- $\frac{1}{2}$ model with weak coupling between planes.

If there is really long-range order in the ground state of the square lattice, it is, nonetheless, of interest to ask if the RVB state is the ground state of *any* unfrustrated two-dimensional lattice. Since corrections to spin-wave theory are largest for small coordination number, the RVB is more likely to be the ground state of the honeycomb lattice, which has $z = 3$, the smallest of any simple two-dimensional lattice. We have therefore applied the Monte Carlo techniques of RY to study the ground state of the spin- $\frac{1}{2}$ antiferromagnet on the honeycomb lattice. We also present, in this paper, some further results on the square lattice which were not given in RY. Our principal result is that the staggered magnetisation is finite for *both* lattices with a value close to that predicted by spin-wave theory.

2. The model

The Hamiltonian that we consider is

$$H = \sum_{\langle i,j \rangle} \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j \quad (1)$$

where the $\boldsymbol{\sigma}_i$ are Pauli spin operators on the sites of the lattice. The interactions run over nearest-neighbour pairs only and we have set the exchange constant to unity.

A simple argument following Anderson (1973) suggests that the RVB state is more likely to be the ground state of the honeycomb lattice than the square lattice. One compares the energy per spin of the Néel state, which is considered as the zeroth-order approximation to a long-range ordered state, with the energy of a valence bond (dimer) state, considered as the zeroth-order approximation to the RVB state. The energy of the Néel state is given by

$$\frac{1}{4}E_{\text{Néel}} = -\frac{1}{2}zS^2. \quad (2)$$

The energy of the valence bond state (Anderson 1973), consisting of a dimer covering of the lattice with nearest-neighbour singlet pairs, is given by

$$\frac{1}{4}E_{\text{VB}} = -\frac{1}{2}S(S+1) \quad (3)$$

for all lattices. Hence the Néel state is a better starting point than the VB state for the square lattice but the two states give the same energy for the honeycomb lattice.

To carry out the simulations we mapped a honeycomb lattice of L^2 hexagons into a square lattice of $N = L \times (2L)$ spins with missing bonds as shown in figure 1. Periodic boundary conditions were applied. This mapping allows us to use the same ‘world-line’ Monte Carlo algorithm (Suzuki 1976, Barma and Shastry 1978, Hirsch *et al* 1982, Marcu 1987) that RY used for the square lattice. In this algorithm one divides the Hamiltonian into two pieces, H_1 and H_2 , where H_1 and H_2 each incorporate the Hamiltonian of every fourth square, as shown in figure 1, in such a way that each bond on the lattice is included in either H_1 or H_2 . The matrix elements of either H_1 or H_2 can be computed separately

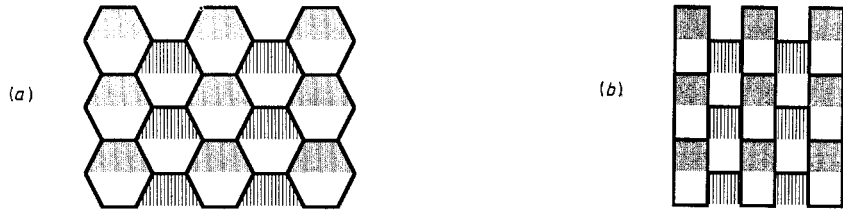


Figure 1. (a) The honeycomb lattice. (b) The equivalent square lattice with missing bonds obtained by distorting (a). We also show the checkerboard break-up of the Hamiltonian into two pieces H_1 (shaded) and H_2 (striped).

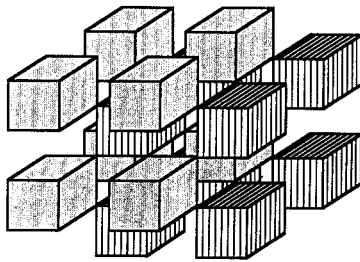


Figure 2. The three-dimensional lattice on which one simulates an effective classical problem. The 'time' direction is vertical. At each lattice point there is a variable taking values ± 1 , which indicates whether the spin is up or down. The statistical weight of a given configuration is the product of matrix elements of $\exp(-\Delta\tau H_{sq})$, where H_{sq} is the Hamiltonian of a single square with a missing bond, between the states of the top and bottom squares of the shaded cubes. H_1 acts in the shaded cubes and H_2 in the striped cubes, similar to figure 1.

because they each split into Hamiltonians of non-interacting squares. Since H_1 and H_2 do not commute, one uses the Trotter formula (Suzuki 1976)

$$\exp(-\beta(H_1 + H_2)) = \lim_{m \rightarrow \infty} \left[\exp\left(\frac{-\beta H_1}{m}\right) \exp\left(\frac{-\beta H_2}{m}\right) \right]^m \quad (4)$$

where $\beta = T^{-1}$, to compute the partition function and expectation values. Inserting complete sets of eigenstates of S^z between the different factors, one sees that the partition function becomes that of a classical model in one higher dimension, with $2m$ 'time slices' in the 'time' or 'Trotter' direction. Periodic boundary conditions must be applied in this direction to represent the fact that a trace is being taken. At each site there is an Ising-like variable that takes values ± 1 and describes whether the spin is up or down. Representing the three-dimensional lattice as in figure 2, the statistical weight of a given spin configuration is simply the product of matrix elements of $\exp(-\Delta\tau H_{sq})$ for each shaded cube, where $\Delta\tau = \beta/m$ and H_{sq} is the Hamiltonian of a single square with a missing bond.

The expectation value of any operator, A , which conserves the total z-component of spin between the two time slices of a single cube, is given by

$$\langle A \rangle = \sum_c A_c P_c \quad (5)$$

where c denotes a configuration of the spins at all time slices, A_c is the value of A in this configuration at any one time slice, and P_c is the probability of a particular configuration. In the Monte Carlo method one takes a statistical sample of the spin configurations using standard techniques (see e.g. Binder 1984), which generate configurations with probability P_c . Note that the Hamiltonian conserves the total magnetisation, M^z , which is therefore the same at each time slice. The ground state, which is our principal interest, has $M^z = 0$ so the simulation is restricted to this subspace.

As discussed by RY, the elementary move is to flip the spins of the four interacting cubes that are nearest neighbours to a non-interacting cube, in such a way that M^z is conserved. With just this move, however, the algorithm does not sample all configurations with $M^z = 0$, so two other moves have been included. The first of these causes the 'world-lines' for two up spins, say, to twist around each other. The second, a non-local move, is included to generate states of different 'winding number' (see e.g. Marcu 1987). As in RY, inclusion of the non-local moves makes a substantial difference to the results for small systems. For the larger sizes, the difference appears to be smaller and the acceptance rate for this type of move becomes very low. However, we have included non-local moves for *all* sizes, performing one sweep of each of the three types of move in turn.

We are interested in computing the staggered magnetisation as would be measured, for example, by neutron scattering or, equivalently, computed from spin-wave theory. However, in these situations the symmetry is spontaneously broken, which does not occur in finite systems. To determine the order parameter from a finite system, the correct procedure, in principle, is to apply a small field that couples to the staggered magnetisation, and to let this field tend to zero after the thermodynamic limit has been taken. In practice this cannot be done because the range of sizes studied is too small. Instead one argues, as for transitions in classical systems at finite temperature, that the probability distribution of the staggered magnetisation can only depend on its magnitude, not on its direction, because the Hamiltonian is rotationally invariant. For a large system the distribution will be very strongly peaked at a particular value of the magnitude. The effect of the symmetry-breaking field is to break the degeneracy with respect to direction and to make the distribution strongly peaked at the same magnitude it had without a field (if the field is small) and a direction determined by the field. Hence one can estimate m^\dagger from rotationally invariant correlation functions for a finite system without a field by recognising that the ground state has long-range order with a given magnitude of m^\dagger , but averaged over all possible directions that this order can have.

As an example, the staggered magnetisation can be deduced from the mean square staggered magnetisation, defined by

$$S(\mathbf{q}_c) = \frac{1}{N^2} \left\langle \left(\sum_{x,y} \tilde{S}^z(x,y) \right)^2 \right\rangle \quad (6)$$

where $\mathbf{q}_c = (\pi, \pi)$ is the wavevector of the staggered magnetisation, x and y are the coordinates of a site on the lattice, and

$$\tilde{S}^z(x,y) = \frac{1}{2} \varepsilon_{x,y} \sigma^z(x,y) \quad (7)$$

where $\varepsilon_{x,y}$ is +1 or -1 depending on which sublattice the site (x,y) lies. The staggered

magnetisation can also be obtained from the correlation between spins as far apart as possible on the lattice, i.e.

$$C_{L/2} = \frac{1}{N} \sum_{x,y} \langle \tilde{S}^z(x, y) \tilde{S}^z(x + L/2, y + L) \rangle. \tag{8}$$

For $L \rightarrow \infty$, where contributions from short-range order can be neglected, both $S(\mathbf{q}_c)$ and $C_{L/2}$ reduce to $(m^\dagger)^2/3$, the factor of 3 appearing from the rotational invariance of the ground state discussed above. Hence we have

$$m^\dagger = \langle \tilde{S}_i^z \rangle = \lim_{L \rightarrow \infty} \sqrt{3S(\mathbf{q}_c)} = \lim_{L \rightarrow \infty} \sqrt{3C_{L/2}}. \tag{9}$$

3. Some technical aspects

To verify that the simulations are in equilibrium, we started the simulation both from an ordered (Néel) state and a completely random initial state (the same at each time slice). For each size we did this for a (roughly) logarithmically increasing set of values of the number of sweeps (increasing both the equilibration sweeps and the subsequent sweeps where measurement takes place). For each size, we verified that the results from the Néel start and the random start were independent of the simulation time for the longer runs and, furthermore, that they agreed with each other within the statistical errors. For $L = 8$ ($N = 128$), which demanded the most computer time, we did one run with 100 000 sweeps (of each of the three types of move) for equilibrium followed by 600 000 steps for the averaging. These were carried out both for a random and a Néel start. In addition, many shorter runs were performed. We performed similar sets of runs for several different values of $\Delta\tau$, as discussed below.

Three extrapolations have to be made to compute the value of m^\dagger in the ground state. Firstly, one has to let the temperature T tend to zero. Taking into account the behaviour of various quantities with respect to temperature observed for the square lattice in RY, we have assumed that $\beta = T^{-1} = 10$ is sufficiently large to guarantee that the results are independent of T . Support for this comes from the work of Barnes *et al* (1988), who find that the energy gap between the singlet ground state and lowest triplet excited state is $\approx 8.4/L$ for the square lattice. Hence our choice of $\beta = 10$ should be sufficiently large, provided the gap behaves in a similar way for the honeycomb lattice.

Secondly, one has to take the limit $\Delta\tau \rightarrow 0$, otherwise errors are made in the use of the Trotter formula equation (4). The error in calculating expectation values is proportional to $\Delta\tau^2$ (Fye 1986, Suzuki 1985). To show this behaviour, we plot in figure 3 the values of the energy for $L = 4$ against $\Delta\tau^2$ together with a quadratic fit. For $L = 4$, we took $\Delta\tau$ equal to 0.20, 0.15625, 0.125, 0.10 and 0.05; for $L = 6$, the values of $\Delta\tau$ were 0.20, 0.15625, 0.125 and 0.10; and for $L = 8$ we considered $\Delta\tau$ equal to 0.15625, 0.125 and 0.10. In addition to these sizes we also have data obtained by exactly diagonalisation the 2×4 lattice.

The final extrapolation is, of course, to infinite system size. We can determine the form of the leading finite-size dependence by assuming that spin-wave theory is *qualitatively* correct. Standard arguments (e.g. Kittel 1963) then show that the transverse spin-spin correlation varies as k^{-1} where k is the wavevector. Fourier transforming gives an r^{-1} dependence in real space in two dimensions. It is also easy to show that the longitudinal correlation function varies as the square of this, i.e. r^{-2} . Since the ground

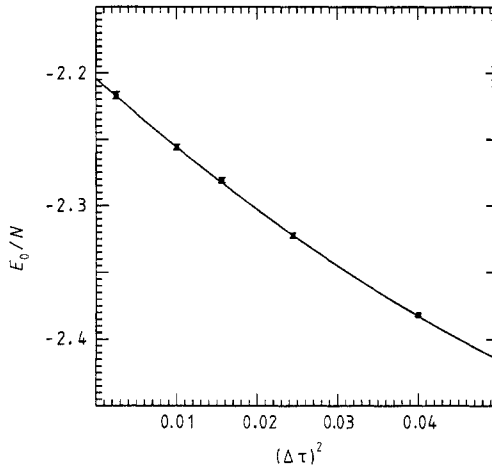


Figure 3. A plot of the energy against $\Delta\tau^2$ for the honeycomb lattice with $L = 4$. A quadratic fit to the data is also shown.

state is rotationally invariant, the S^z – S^z correlation function is a linear combination of the longitudinal and transverse correlation functions. Hence the transverse part is dominant at long distances and so we have

$$\langle \tilde{S}_i^z \tilde{S}_j^z \rangle - (m^+)^2/3 \sim 1/r_{ij}. \quad (10)$$

As a result, the leading finite-size correction to $S(\mathbf{q}_c)$ and $C_{L/2}$ varies as $1/L$ (RY, Huse 1988).

It is also useful to obtain this result in a different way. We are effectively interested in the difference between the Brillouin zone integrals in spin-wave theory and the corresponding sums that arise in calculations on a finite system. The leading finite-size dependence comes from the singularity in the integrand at $k = 0$ due to the $\omega \propto k$ spin-wave dispersion. Since the $k = 0$ point is just one out of L^2 allowed k -values this would naively give a L^{-2} finite-size correction. However the contribution of a mode of wavevector k to $S(\mathbf{q}_c)$ diverges as k^{-1} , so the naive contribution has to be multiplied by the contribution of the longest wavelength spin wave that can fit in the system, i.e. the inverse of $k_{\min} (\sim L^{-1})$. This leads to the L^{-1} finite-size correction for $S(\mathbf{q}_c)$ and $C_{L/2}$. Applying the same argument to the ground-state energy yields a finite-size correction of L^{-2} multiplied by the energy of the spin wave of wavevector k_{\min} . This gives an L^{-3} correction (Huse 1988), so the energy converges much more rapidly than the staggered magnetisation.

4. Results

First of all we present our results for the energy. The ground-state energy of the hexagonal lattice is plotted for several sizes in figure 4, which clearly shows the L^{-3} variation. From the fit shown in the figure we obtain

$$E_0 = -2.178 \pm 0.005 \quad (\text{honeycomb}) \quad (11)$$

in units of the interaction constant. From equation (2) we see that $E_0/E_{\text{Néel}} =$

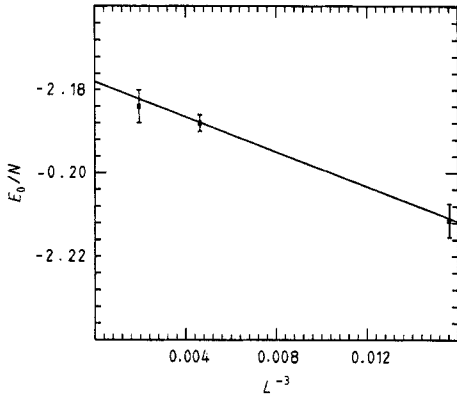


Figure 4. A plot of the ground-state energy of the honeycomb lattice against L^{-3} with sizes between $L = 4$ and $L = 8$. A linear fit to the data is also shown.

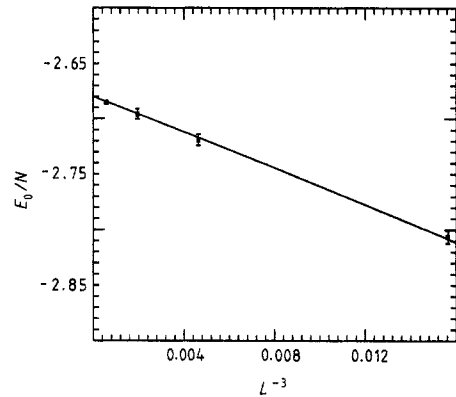


Figure 5. A plot of the ground-state energy of the square lattice against L^{-3} for sizes between $L = 4$ and $L = 12$. The curve is a quadratic fit, which also passes through the data point for $L = 2$ (not shown).

1.452 ± 0.003 . Our result is somewhat lower than the spin-wave value (Dimino 1988) of -2.144 . Oitmaa and Betts (1978) found -2.112 , in our units, by exact diagonalisation of clusters of up to 18 spins. However, they extrapolated to the thermodynamic limit assuming an L^{-2} size dependence, which accounts for the discrepancy with our result.

For the square lattice, RY quoted a ground-state energy value of -2.680 ± 0.008 . We have since done a more careful study and show the results in figure 5. The extrapolation gives

$$E_0 = -2.680 \pm 0.002 \quad (\text{square}) \quad (12)$$

which can be reexpressed as $E_0/E_{\text{Néel}} = 1.340 \pm 0.001$.

As for the honeycomb lattice, we believe that the result of Oitmaa and Betts (1978), that $E_0 = -2.62 \pm 0.02$, is somewhat high because they extrapolated assuming an L^{-2} size dependence. The energy in equation (12) is consistent with the value -2.676 ± 0.004 obtained by Barnes *et al* (1988) but is in definite disagreement with Gross *et al* (1988) who find -2.669 ± 0.0011 . Because of this discrepancy we checked more carefully that the temperature was low enough in our calculations. For the square lattice we repeated the runs for $L = 8$ with $\Delta\tau = 0.1$ and 0.05 using $\beta = 25$, compared with $\beta = 10$ used previously. In addition, we repeated the run for $L = 12$ and $\Delta\tau = 0.1$ using $\beta = 40$ compared with $\beta = 15$. In all cases the new results agreed with our old values to within the error bars. We are therefore confident that our calculations describe the zero-temperature limit. The variational estimate of Huse and Elser (1988) that $E_0 = -2.6552$ is clearly very close to the correct answer (less than 1% too high according to our result).

In figure 6, we display our main results for $S(\mathbf{q}_c)$ and $C_{L/2}$ for the honeycomb lattice, together with a quadratic fit to the data. The extrapolated values of $S(\mathbf{q}_c)$ and $C_{L/2}$, which should be equal, are indeed very close, the fit giving 0.0154 and 0.0166 respectively. This should be compared with the saturation value of $\frac{1}{12}$. From equation (9) we find

$$m^\dagger = 0.22 \pm 0.03 \quad (\text{honeycomb}) \quad (13)$$

or, in other words, 44% of the saturation value. The error was estimated from the range

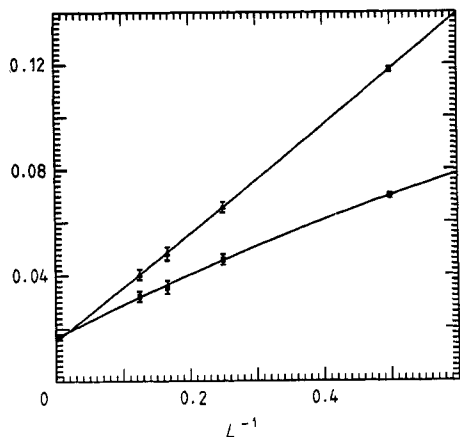


Figure 6. A plot of $S(q_c)$ (triangles) and $C_{L/2}$ (squares) against L^{-1} for the honeycomb lattice. The curves are quadratic fits to the data.

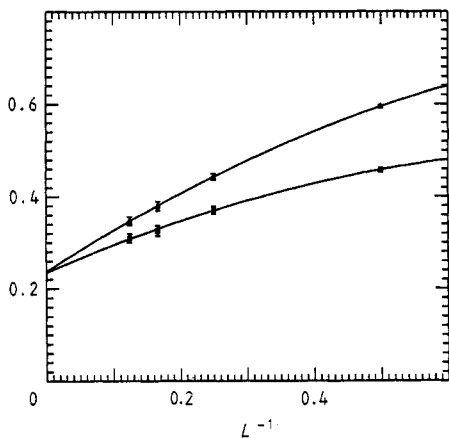


Figure 7. A plot of $\sqrt{3S(q_c)}$ (triangles) and $\sqrt{3C_{L/2}}$ (squares) against L^{-1} for the honeycomb lattice. The intercept is equal to m^\dagger . The curves are quadratic fits to the data.

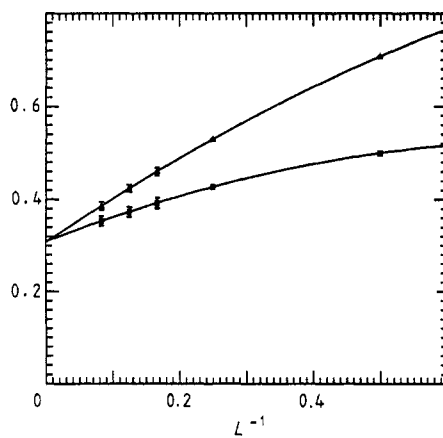


Figure 8. A plot of $\sqrt{3S(q_c)}$ (triangles) and $\sqrt{3C_{L/2}}$ (squares) against L^{-1} for the square lattice. The intercept is equal to m^\dagger . The curves are quadratic fits to the data.

of quadratic fits which gave a reasonable description of the data. Interestingly, our value for m^\dagger agrees, within the error bars, with the spin-wave estimate (Dimino 1988) of 0.242. We will comment on this further in the conclusions below. Our extrapolated value of $S(q_c)$ disagrees with the Oitmaa and Betts (1978) prediction of 0.054 ± 0.003 because they used an L^{-2} extrapolation. Furthermore, they omitted the factor of 3 in equation (9) which determines m^\dagger in terms of $S(q_c)$. Our value of m^\dagger is, as expected, lower than the corresponding for the square lattice

$$m^\dagger = 0.30 \pm 0.02 \quad (\text{square}) \tag{14}$$

(60% of the saturation value) given by RY.

We have also plotted $\sqrt{3S(q_c)}$ and $\sqrt{3C_{L/2}}$, which give m^\dagger directly, against $1/L$ and show the results for the honeycomb lattice in figure 7. The extrapolated value of 0.235 ± 0.028 is close to the result in equation (13) obtained by extrapolating the square

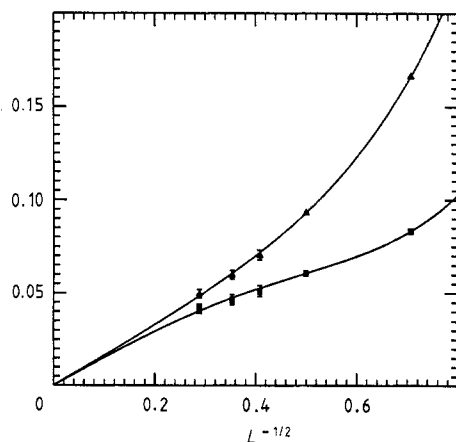


Figure 9. A plot of the data of RY for $S(q_c)$ (triangles) and $C_{L/2}$ (squares) for the square lattice against $L^{-1/2}$. Unlike Miyashita (1988), we are unable to fit our data to $aL^{-x}(1 + b/N)$, with x close to $\frac{1}{2}$ and the curves shown are fits to $aL^{-1/2}(1 + b/N + c/N^2)$.

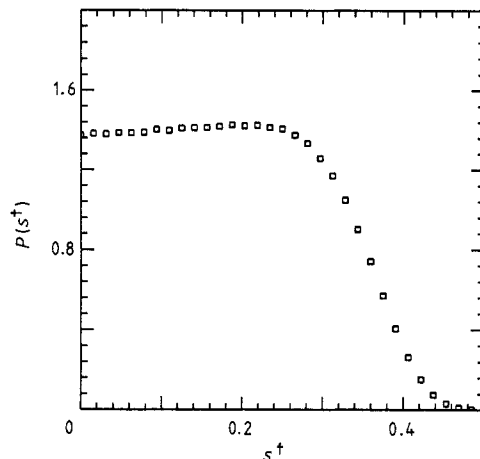


Figure 10. The probability distribution of the staggered magnetisation, s^\dagger , in the ground state of the honeycomb lattice for $L = 8$ and $\Delta\tau = 0.125$. Since the distribution is symmetric we only show the region for s^\dagger positive.

of this quantity. For comparison we present the analogous plot for the square lattice in figure 8, using the data of RY. The extrapolated value of 0.308 ± 0.015 agrees well with the earlier estimate given by RY of $m^\dagger = 0.30 \pm 0.02$. Given the uncertainties in the extrapolations, which are hard to estimate reliably, we do not feel that there is any significance in the difference between the results for the square lattice of RY and those of Tang and Hirsch (1988), who find 0.25 ± 0.03 . In a very careful study, Gross *et al* (1988) find $m^\dagger = 0.285 \pm 0.015$ in agreement with RY. The numerical results of Horsch and von der Linden (1988) are consistent with RY but their quoted value for m^\dagger is different because they omit the factor of 3 in equation (9), for reasons which are unclear to us.

In contrast to our conclusions, Miyashita (1988) has suggested, on the basis of data for $S(q_c)$ for the square lattice with sizes up to $L = 10$, that $S(q_c)$ vanishes as $L^{-0.48}$ as $L \rightarrow \infty$. To investigate this possibility, we plot in figure 9 the data of RY for the square lattice against $1/\sqrt{L}$. We see that our results for $C_{L/2}$, apparently not calculated by Miyashita, would have an 'S'-shaped curve if the data is really extrapolating to zero in the thermodynamic limit. We feel that this is unlikely and note further that there is no theoretical reason for the $L^{-1/2}$ behaviour, unlike our extrapolation which is based on spin-wave theory. We shall discuss this further in the conclusions below.

We commented above that the ground state has a fixed magnitude of the staggered magnetisation (at least for large systems) but that all directions are averaged over. To illustrate this directly, we plot in figure 10, the distribution of the z-component of the staggered spin, $P(s^\dagger)$, where s^\dagger , the staggered spin per site, is defined by $s^\dagger = N^{-1} \sum_i \hat{S}_i^z$. If the ground state has long-range order, this should be a uniform distribution, since it is simply the distribution of $\cos \theta$ over a sphere. The plot clearly shows a rectangular distribution, with some finite-size rounding, and no evidence for peaking at small values of s^\dagger , which would be expected if m^\dagger were zero. Note that $S(q_c)$ is just the second moment of $P(s^\dagger)$. We have also obtained similar results for the square lattice.

Similar results and conclusions for the distribution of the order parameter have also been reached by Tang and Hirsch (1988).

5. Conclusions

We have shown that the staggered magnetisation in the spin- $\frac{1}{2}$ antiferromagnet on the honeycomb lattice is finite and is, furthermore, quite close to the spin-wave value. Similar results have been found earlier by RY for the square lattice. Our numerical values are given in equations (13) and (14) for the honeycomb and square lattices respectively.

An interesting question, which these results raise, is why spin-wave theory should be so accurate. Oguchi (1960) showed that the next term in the spin-wave expansion vanishes for any lattice with inversion symmetry, such as the square lattice, though the correction will be non-zero for the honeycomb lattice. Our results show that the coefficient of this term for the honeycomb lattice must be small, as must the coefficient of the next-order term for both lattices. It would be clearly useful to investigate the expansion in more detail, to understand why the leading term works so well.

Our quoted errors assume that the leading finite-size correction to $S(\mathbf{q}_c)$ and $C_{L/2}$ varies as L^{-1} , which comes from the spin-wave prediction of an r^{-1} decay of the staggered spin correlations to their asymptotic value, see equation (10). We cannot completely rule out the possibility that these correlations tend to zero at infinite distance with some small inverse power of L . However, one would then need substantial corrections to this asymptotic behaviour to force the fit through the data. There is, however, no theoretical reason for such behaviour as far as we can see. Even in a situation where quantum fluctuations drive the system to the zero-temperature critical point described by Chakravarty *et al* (1988), the correlations still decay to zero like r^{-1} (neglecting the small exponent η of the three-dimensional classical Heisenberg magnet). Hence our extrapolation with size would *still* be correct. Actually, as mentioned in reference [15] of Chakravarty *et al* (1988), the model they use does not distinguish between integer and half-integer spin, so there is some question as to whether it gives the correct description of the quantum-disordered phase. Hence this argument cannot be regarded as completely sound. Nonetheless, there is, to our knowledge, no theory which predicts a lack of long-range order and which is compatible with our data. We therefore feel reasonably confident that our extrapolations are correct.

We also note that additional support for the accuracy of spin-wave theory comes from the good agreement between the measurements of Endoh *et al* (1988) on the magnetic correlation length of La_2CuO_4 and the theory of Chakravarty *et al* (1988). Furthermore the largest staggered magnetisations observed in La_2CuO_4 are close to the spin-wave estimate of $\approx 0.6\mu_B$ per site (Shirane *et al* 1987, Vaknin *et al* 1987).

Finally, although we have argued that the RVB state is not the ground state of the square or honeycomb lattices, it is possible that RVB states with relatively low energy may give a contribution to the low-temperature thermodynamic properties. This is currently under investigation.

Acknowledgments

We benefitted from discussions with R N Bhatt and S Chakravarty. This work was supported by the NSF through grants DMR 84-19536 and DMR 85-10593. JAR is

financially supported with by the Consejo Nacional de Investigaciones Científicas y Técnicas de la Argentina. The computations were done on a Culler-7 minicomputer and Sun workstations.

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