Dimer versus Twist Order in the J_1-J_2 Model

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(Received 6 June 1990)

We diagonalize fully the 4×4 $S=\frac{1}{2}$ Heisenberg model with nearest-neighbor (J_1) and second-neighbor (J_2) exchanges for several values of J_2/J_1. For $J_2/J_1\approx 1/2$ the specific heat shows a peak near $T=0.27J_1$, and the dimer order increases sharply around that temperature. In contrast, the twist order considered earlier by Dagotto and Moreo drops below that temperature, and its $T=0$ value is roughly the same as that at $T=\infty$. This shows that while the system may develop long-range dimer order (and it certainly has appreciable short-range dimer order) for these values of J_2/J_1, there is no indication of enhanced twist order.

PACS numbers: 75.10.Jm, 74.65.+n, 75.40.Mg

Motivated by the discovery of antiferromagnetism in the insulating phase of high-T_c materials and the suggestion[1] that magnetic fluctuations may be central to a microscopic understanding of the high-T_c phenomena, there have been several theoretical studies of ground-state properties of frustrated square-lattice Heisenberg models. Perhaps the simplest of these models is the J_1-J_2 model, with nearest-neighbor antiferromagnetic exchange J_1 and the second-neighbor exchange J_2. In the classical limit ($S\rightarrow\infty$), this model has a two-sublattice Néel ground state for $J_2/J_2<1/2$ and a four-sublattice Néel ground state for $J_2/J_1>1/2$. At $J_2/J_1=1/2$ various states ordered at wave vectors (π,q), or (q,π), become degenerate. Expansion in powers of $1/S$ reveals[2] that the magnetically ordered phases are pulsed away from $J_2/J_1=1/2$ leaving an intermediate phase with no long-range magnetic order. The nature of the ground state in this intermediate phase has been of considerable interest.

Chandra and Doucot[2] in their $1/S$ expansion suggested that the ground state in the intermediate phase was a resonating-valence-bond (RVB) state with no long-range order. Based on a large-N expansion, Read and Sachdev[3] suggested that the magnetically disordered phase obtained by quantum fluctuations may have long-range dimer order, where the nearest-neighbor spin correlations alternate in a column pattern. Other suggestions have included twist order[4] as well as chiral order.[5] For $S=\frac{1}{2}$, numerical studies have proven very useful for understanding the unfrustrated ($J_2=0$) Heisenberg model.[6] Many of them have been applied to the frustrated case as well. Series-expansion studies of Gelfand, Singh, and Huse[7] provided estimates of the magnetic phase boundaries and presented evidence for dimer order in the intermediate phase, in agreement with the suggestion of Read and Sachdev. The symmetries of the low-lying states for the 4×4 system also indicate dimer order.[7] However, the analysis of the same 4×4 system led Figueirido *et al.*[8] to conclude an RVB phase with only short-range dimer order. Since in the series

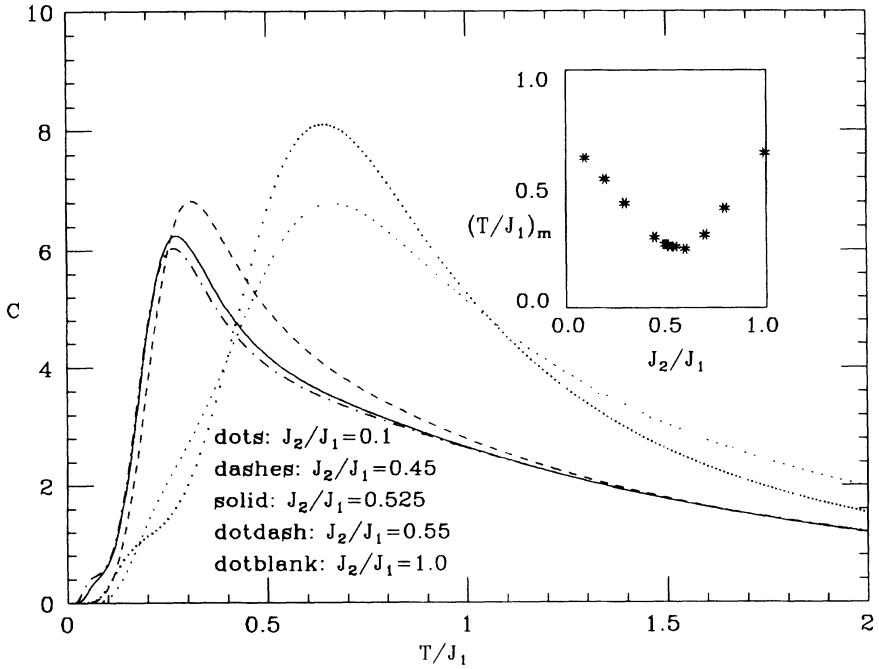

FIG. 1. Plots of specific heat vs temperature for various values of J_2/J_1. Inset: Location of the peaks as a function of J_2/J_1.

analysis only a few terms were used, and in the finite system studies only very small systems were considered, the question of long-range order is difficult to settle. By way of comparison, it should be noted that in the series analysis an extrapolation to an infinite series was attempted, whereas no analogous extrapolation was done in the study of finite systems. Recently, Gelfand has further extended the series study,[9] where he considered various types of dimer patterns and concludes that the system is ordered in the columnar pattern, but the value of the order parameter may be small compared to its maximal value.

In contrast to these studies, the numerical studies of Dagotto and Moreo[10] raised the possibility of another type of order, namely, twist order. They studied the ground state of the 4×4 and $\sqrt{20}\times\sqrt{20}$ systems and evaluated the square of various order parameters in those systems. These included dimer, twist, and chiral order parameters. By studying the variation of these order parameters with J_2 they found that while the chiral order parameter showed no sign of enhancement both the dimer and twist order parameters had a peak around $J_2/J_1 \approx 1/2$. Furthermore, the peak for the dimer order parameter decreased in magnitude as one went from the 16- to 20-site system, while it sharpened and increased in magnitude for the twist order parameter. From this they concluded that the twist order is strongly enhanced in the intermediate phase. This result has since been repeatedly emphasized in the literature[11] as an evidence for twist order in the J_1-J_2 model. An important ingredient missing from their analysis is the finite-temperature value of these quantities, and how the zero-temperature results at various J_2/J_1 compare with that value.

In this paper we study the 4×4 periodic system at finite temperatures by a complete diagonalization. We study the specific heat, the static structure factors, as well as the squares of dimer and twist order parameters. The thermal expectation values of the squares of the dimer and twist order parameters are[12]

$$\psi = \frac{\sum_m \langle m|2[N^{-1}\sum_{i_x,i_y}(-1)^{i_x}\mathbf{S}_i\cdot\mathbf{S}_{i+\hat{x}}]^2|m\rangle e^{-\beta E_m}}{\sum_m e^{-\beta E_m}} \equiv \frac{\sum_m \psi_{mm} e^{-\beta E_m}}{\sum_m e^{-\beta E_m}}, \quad (1)$$

$$\phi = \frac{\sum_m \langle m|[N^{-1}\sum_{i_x,i_y}\mathbf{S}_i\times(\mathbf{S}_{i+\hat{x}}+\mathbf{S}_{i+\hat{y}})]^2|m\rangle e^{-\beta E_m}}{\sum_m e^{-\beta E_m}} \equiv \frac{\sum_m \phi_{mm} e^{-\beta E_m}}{\sum_m e^{-\beta E_m}}. \quad (2)$$

Here, $|m\rangle$ are the energy eigenstates with energies E_m at a particular value of J_2/J_1. In order to carry out our studies, it was sufficient to diagonalize the $S^z_{\rm tot}=0$ subspace, and determine the total spin of each of these states. In addition, certain symmetries of the lattice were used to block diagonalize the Hamiltonian. The details have been discussed elsewhere.[13]

We find that in the intermediate region around $J_2/J_1=1/2$ the specific heat of the system has a peak around a temperature of $0.27J_1$. Near this temperature the square of the bond order parameter ψ increases sharply as the temperature is lowered. Between a temperature of $0.5J_1$ and $0.1J_1$ it increases by roughly a factor of 2.5. The zero-temperature value of ψ is roughly 0.4 times that of a fully dimerized state. This is a clear evidence for enhancement of dimer order. In contrast, the square of the twist order parameter ϕ does not show any significant enhancement with respect to the infinite-temperature value. The only structure is a maximum increase of about 20% between $T=\infty$ and $T\approx 0.27J_1$, which is followed by a decrease as the temperature is further lowered. Hence, there is no indication of twist order at $T=0$. In light of this, the results of Dagotto and Moreo with regards to the twist order parameter need to be reinterpreted. At infinite temperature all states occur with equal probability. Thus, the value of the order parameter at $T=\infty$ is just the average over all states, and is independent of J_2/J_1. The fact that Dagotto and Moreo found a peak in the twist order parameter at $T=0$ as a function of J_2/J_1 is simply because this order parameter is strongly suppressed in the magnetically ordered phases. This result is apparent if one looks at the operator itself in (2). In the four-sublattice Néel phase ($J_2/J_1 \gg 1/2$) the $\mathbf{S}_{i+\hat{x}}+\mathbf{S}_{i+\hat{y}}$ factors in the twist order parameter tend to cancel each other. In the two-sublattice Néel phase ($J_2/J_1 \ll 1/2$) the neighboring spins align antiparallel, and hence their cross product is small. Indeed, the twist order parameter in the intermediate region at $T=0$ is the typical value in a randomly chosen state, and is hardly different from that at $T=\infty$.

In Fig. 1 the specific heat of the system is plotted for different values of J_2/J_1. There are two things to notice. The peak in the specific heat sharpens in the intermediate region. Second, the peak position plotted as a function of J_2/J_1 flattens out between $0.4 < J_2/J_1 < 0.7$ (see inset). For small J_2/J_1, one does not expect any finite-temperature transition. Thus, the peak there represents the gradual ordering of the systems into the antiferromagnetic ground state. If the order parameter in the intermediate region has a discrete symmetry, as in case of dimer order, one would expect a finite-temperature phase transition there. The sharpening of the peak in that region is consistent with such a possibility. Clearly the 4×4 system is too small to decide between a gradual ordering into a zero-temperature state and a finite-temperature transition.

The analysis of the structure factors showed the expected behavior. In the region of small J_2/J_1 the structure factor at wave vector (π,π) was considerably enhanced, indicating a two-sublattice Néel order. For

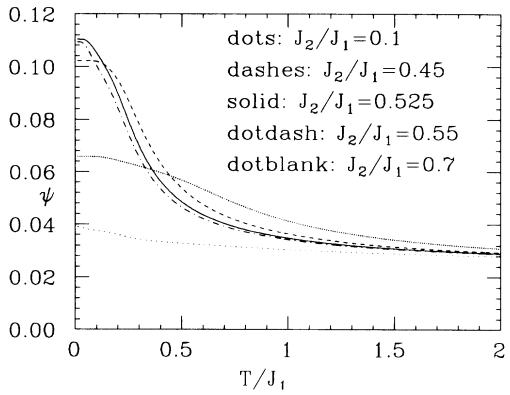

FIG. 2. Plots of the square of the dimer order parameter vs temperature for various values of J_2/J_1.

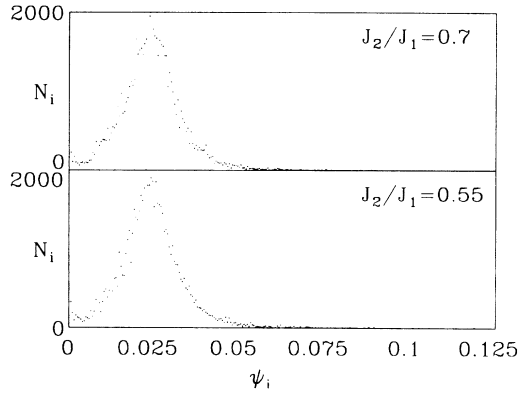

FIG. 3. The distribution of the expectation value of the square of the dimer order parameter in the energy eigenstates for $J_2/J_1=0.55$ and 0.7.

large J_2/J_1 the structure factor at wave vector $(0,\pi)$ was enhanced indicating a four-sublattice Néel order. In the intermediate region there was no significant enhancement of magnetic order at any wave vector.

In Fig. 2 we show the dependence of the dimer order parameter on temperature for different values of J_2/J_1. Clearly this order parameter is strongly enhanced at low temperatures with respect to a typical value in the intermediate region (around $J_2/J_1=1/2$). Let us group the energy eigenstates $|m\rangle$ into bins so that all the states in one bin have a value of ψ_{mm} [see (1)] in a small range with the central value being different for different bins. Let N_i denote the total number and ψ_i the central value in bin i. The plot of N_i vs ψ_i for two different values of J_2/J_1 is shown in Fig. 3. The mean of this distribution is the infinite-temperature expectation value of ψ and is independent of J_2/J_1. However, the plots show that the entire distribution is hardly altered by changing J_2/J_1. The possible invariance of this distribution in the thermodynamic limit may be related to properties of random matrices and deserves further attention. We find that the mean of the distribution is 0.023 and the standard deviation is 0.009. At $J_2/J_1=0.525$ the zero-temperature value of ψ is 0.11 which is 10 standard deviations away from the mean value. Therefore, there is a large enhancement in the intermediate region. This shows that at low temperatures the behavior is dominated by the tails of the distribution and that the low-energy states are special with regard to the dimer operator. The value of ψ at $T=0$ is roughly 0.4 times that in a fully dimerized state which corresponds to the order parameter attaining a value of 0.6 times its maximum. However, without considering the systematic size dependence of this quantity we cannot establish the presence or absence of long-range order.

In Fig. 4 we show the dependence of the twist order parameter on temperature for different values of J_2/J_1. In the intermediate region, this order parameter is hardly different at low temperatures from its infinite-temperature value. Its decrease, near the temperature where the specific heat shows a maximum, is analogous to the behavior of the uniform susceptibility in an antiferromagnet,[14] which simply suggests that it is some other quantity that orders. A distribution similar to the one discussed for the dimer order parameter in the previous paragraph was constructed for the twist order parameter. This is plotted in Fig. 5 for two different values of J_2/J_1. We find, once again, that the central features of this distribution are unchanged as one changes J_2/J_1. The mean value of the square of the twist order parameter is 0.047 with a standard deviation of 0.0105. Thus, the zero-temperature value, even at $J_2/J_1=0.5$, where Dagotto and Moreo find the maximum at $T=0$, is within a standard deviation of the mean value. Thus, there is nothing special in the states that dominate at low temperatures as far as this order parameter is concerned. In the magnetically ordered regions, this order parameter is unusually low, as it gets anticorrelated. For small J_2/J_1 the nearest-neighbor spins align collinearly; hence their cross product is suppressed. For large J_2, the twist order parameter as defined in (2) is strongly suppressed as the neighboring spins on a given sublattice order antiparallel; hence $\mathbf{S}_{\mathbf{i}+\hat{\mathbf{x}}}+\mathbf{S}_{\mathbf{i}+\hat{\mathbf{y}}}$ tend to cancel each other.

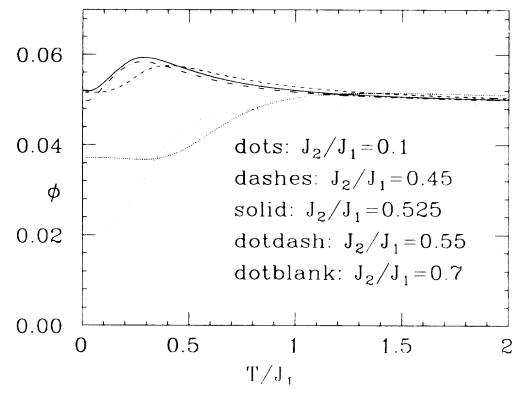

FIG. 4. Plots of the square of the twist order parameter vs temperature for various values of J_2/J_1.

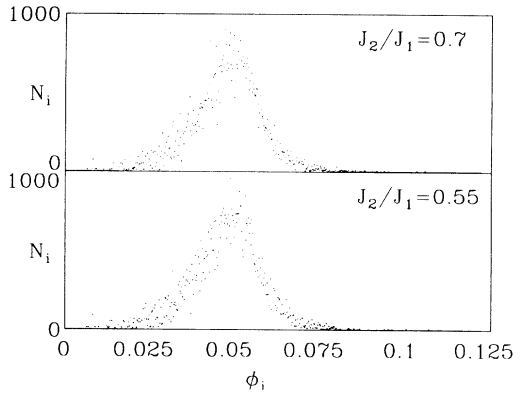

FIG. 5. The distribution of the expectation value of the square of the twist order parameter in the energy eigenstates for $J_2/J_1=0.55$ and 0.7.

A complete diagonalization of the 20-site system has not been attempted.[15] We would like to make three comments regarding the difference between the results of 16- and 20-site systems in the study of Dagotto and Moreo. First, the difference is too large considering the small change in the linear dimension of the system to indicate any systematic size-dependent trends. It primarily reflects the fact that both dimer and twist order parameters have very large unit cells and hence are extremely sensitive to changes in shapes for such small systems. Second, Gelfand has shown[9] that the magnetic and dimer correlation lengths are at least two or three lattice spacings in the region of interest; thus, in the 16- or 20-site systems with periodic boundary conditions, where the maximum distance between the spins is only three to four spacings, there are bound to be large finite-size effects. And third, on very general grounds one expects the square of the order parameter to decrease to its infinite-size limit as the size of the system is increased. This is because the square of the order parameter is an average over short-range order and long-range order. In a finite system it is always nonzero because the short-range order is nonzero. In the infinite system, the short-range part has zero weight relative to the long-range part. Thus, this becomes a measure of long-range order, and goes to zero unless the correlations become infinite ranged. As long as correlations decay with distance, the quantity should decrease to its infinite-size limit as the size of the system is increased. Thus, the statement, that the twist order parameter scales with the size of the system whereas the dimer order parameter does not,[11] appears irrelevant.

To conclude, we summarize our results. Studying the 4×4 system at finite temperatures reveals that the J_1-J_2 model may have long-range dimer order at low temperatures for values of J_2/J_1 near $\frac{1}{2}$. It certainly has substantially enhanced short-range dimer order. The growth of this order parameter with temperature is correlated with the peak in the specific heat, possibly indicating a finite-temperature transition. On the other hand, we have demonstrated that the system does not show any appreciable correlations for the twist order for all values of J_2/J_1 in contrast to earlier results. Our studies clearly show that it is not enough to consider the variation of the order parameter with J_2/J_1 at $T=0$ to infer any enhancement of correlations. It is essential to compare the $T=0$ value with that at $T=\infty$. Finally, we note that the distribution of expectation values of the squares of various order parameters may have certain universal properties which deserve further attention.

We are grateful to M. P. Gelfand for comments.

[1]P. W. Anderson, Science **235**, 1196 (1987).

[2]P. Chandra and B. Doucot, Phys. Rev. B **38**, 9335 (1988).

[3]N. Read and S. Sachdev, Phys. Rev. Lett. **62**, 1694 (1989).

[4]P. Chandra, P. Coleman, and A. I. Larkin, Rutgers University report, 1989 (to be published).

[5]X. G. Wen, F. Wilczek, and A. Zee, Phys. Rev. B **39**, 11413 (1989).

[6]R. R. P. Singh, Phys. Rev. B **39**, 9760 (1989); J. D. Reger and A. P. Young, Phys. Rev. B **37**, 5978 (1988).

[7]M. P. Gelfand, R. R. P. Singh, and D. A. Huse, Phys. Rev. B **40**, 10801 (1989).

[8]F. Figueirido *et al.*, Phys. Rev. B **41**, 4619 (1990).

[9]M. P. Gelfand, University of California, Los Angeles, report, 1990 (to be published).

[10]E. Dagotto and A. Moreo, Phys. Rev. Lett. **63**, 2148 (1989).

[11]See, for example, I. Ritchey, P. Chandra, and P. Coleman, Phys. Rev. Lett. **64**, 2583 (1990).

[12]At zero temperature these quantities reduce to those considered by Dagotto and Moreo in Ref. 10. Our calculations reproduce their numbers at $T=0$.

[13]R. Narayanan and R. R. P. Singh, University of California, Davis, Report No. UCD-90-11, 1990 (to be published).

[14]See, for example, R. R. P. Singh and M. P. Gelfand, Phys. Rev. B **42**, 996 (1990).

[15]It can, perhaps, be done on a supercomputer. All our calculations were done on a SUN Sparcstation.