Disorder Induced Phase Transition in a Two-Dimensional Random Quantum Antiferromagnet

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A two-dimensional Heisenberg model with random antiferromagnetic nearest-neighbor exchange is studied using quantum Monte Carlo techniques. As the strength of the randomness is increased, the system undergoes a transition from an antiferromagnetically ordered ground state to a gapless disordered state. The finite-size scaling of the staggered structure factor and susceptibility is consistent with a dynamic exponent $z = 2$.

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The two-dimensional (2D) antiferromagnetic Heisenberg model with nearest-neighbor interactions on a square lattice has been the subject of intense research over the past few years, owing much to its relevance to the physics of the cuprate superconductors [1]. Numerical studies have confirmed that the ground state is ordered [2] with a sublattice magnetization close to the spin-wave theory prediction [3]. By including longer-range frustrating interactions, or by dimerizing the lattice, the system can be driven through an order-disorder transition [4,5]. For a clean system, this phase transition has been argued to be described by the (2 + 1)-dimensional nonlinear sigma model [4,6]. Recent work on this field theory, in particular in the so-called renormalized classical [4] and quantum critical [7] regimes, has led to a detailed understanding of quantum antiferromagnetism in 2D. Numerical studies [8,9] and experiments on the cuprates [10] have confirmed that the theory is quantitatively accurate. In the presence of randomness in the spin-spin interactions, the nonlinear sigma model description is no longer expected to be valid [4,7]. In contrast to the 1D case [11], very few analytic results have been established for higher-dimensional random quantum spin systems [12]. Because of the considerable computational effort required, numerical work has also been quite limited. Recent work has focused on the Ising spin glass in a transverse field [13], and the diluted Heisenberg model [14].

In this paper we report results of extensive quantum Monte Carlo simulations of the $S = \frac{1}{2}$ random exchange model

$$\hat{H} = \sum_{\langle i,j \rangle} J_{ij} \vec{S}_i \cdot \vec{S}_j , \qquad (1)$$

where $\langle i, j \rangle$ is a pair of nearest-neighbor sites on a 2D square lattice. The couplings J_{ij} take two values, $J_{ij} = J(1 \pm \Delta)$, at random, with a probability p for $1 + \Delta$ and $1 - p$ for $1 - \Delta$. We consider only the case $\Delta < 1$, i.e., all couplings are antiferromagnetic and the system is nonfrustrated. We show that there is a parameter regime where the model has a disordered ground state. Results for the uniform susceptibility and the dynamic structure factor show that the disordered phase is gapless. We also study the critical behavior of the order-disorder transition. In particular, using directly the size dependence of the staggered structure factor and the staggered susceptibility, we obtain a dynamic exponent consistent with the value $z = 2$. The critical behavior of this disorder-driven quantum phase transition is thus consistent with the hyperscaling predictions for two-dimensional "dirty bosons" [15], of which our model is a special case.

We study the behavior of the Hamiltonian (1) in the (p, Δ) plane. For $\Delta \to 0$ the clean 2D Heisenberg model is recovered independently of p, and the system is hence ordered at $T = 0$. For $\Delta \to 1$ (but $\Delta \neq 1$) both limits $p \to 0$ and $p \to 1$ correspond to the 2D Heisenberg model with dilute bond impurities. Thus, the system should be ordered in these regimes as well. As p is increased from 0 there will be an increasing fraction of singlets forming at isolated strong bonds in a background of weakly coupled spins. We argue that at a lower critical concentration $p = p_{c1}$ this leads to an order-disorder transition, in analogy with order-disorder transitions due to singlet formation in clean quantum antiferromagnets, such as the two-layer Heisenberg model [9] and various other dimerized models [5]. As p is increased further, there must be another transition to an ordered state at $p = p_{c2}$, as the strong bonds start to dominate and the weak bonds effectively become impurities in a background of strongly coupled spins. As Δ is lowered the tendency to singlet formation diminishes, and one expects the range $[p_{c1}(\Delta), p_{c2}(\Delta)]$ to become smaller and eventually vanish at some $\Delta = \Delta_{\min}$ [16]. Below we present numerical results supporting this picture, which is illustrated by the phase diagram outlined in Fig. 1. The solid circles are results of our quantum Monte Carlo simulations, to be discussed below.

We have used a modification of Handscomb's quantum Monte Carlo technique [17,18] and averaged over 50–300 realizations of the random couplings in order to obtain results useful for extrapolation to the thermodynamic limit. We have studied systems of L^2 spins with periodic boundary conditions. In order to obtain ground state results for $L = 4$–10, we have carried out simulations at inverse temperatures $\beta = J/T$ as large as 128, which for these system sizes is enough for all calculated quantities to have saturated to their $T = 0$ value. A theorem by

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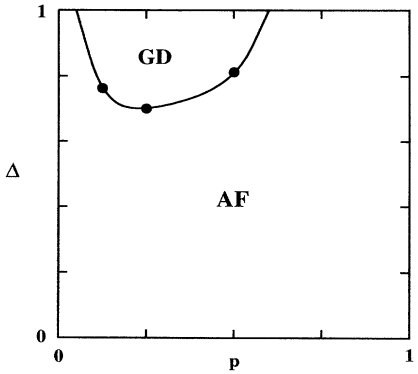

FIG. 1. Proposed phase diagram of the random exchange model (1) in the (p, Δ) plane. The solid circles are Monte Carlo estimates of transition points between the antiferromagnetic (AF) and gapless disordered (GD) phases. The curve is a schematic outline of the rest of the phase boundary, based on the arguments in the text.

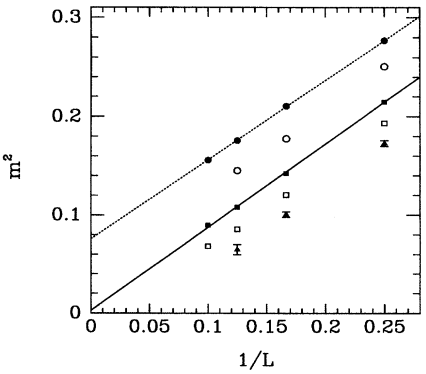

FIG. 2. The sublattice magnetization squared versus the inverse system size at a strong-bond concentration $p = 1/4$ and $\Delta = 0$ (solid circles), $\Delta = 0.5$ (open circles), $\Delta = 0.7$ (solid squares), $\Delta = 0.8$ (open squares), and $\Delta = 0.9$ (solid triangles). Where not shown, statistical errors are smaller than the size of the symbols. The dashed and solid lines are fits to the $\Delta = 0$ and $\Delta = 0.7$ data, respectively.

Lieb and Mattis [19] guarantees that the ground state of a finite system with an even number of spins is a singlet, as long as all couplings are antiferromagnetic (this is not true if $\Delta = 1$, as the lattice then is disconnected). We have therefore restricted the simulations to the subspace with zero magnetization ($\sum_i S_i^z = 0$). We have also studied lattices with $L = 32$ at higher temperatures. In these simulations Monte Carlo moves changing the total magnetization were included.

The sublattice magnetization m for a finite system can be defined according to

$$m^2 = 3S(\pi, \pi)/L^2, \tag{2}$$

where $S(\pi, \pi)$ is the staggered structure factor

$$S(\pi, \pi) = \frac{1}{L^2} \sum_{j,k} e^{i\vec{\pi}\cdot(\vec{r}_j - \vec{r}_k)} \langle S_j^z S_k^z \rangle . \tag{3}$$

For the clean 2D Heisenberg model, spin-wave theory gives the leading size dependence of m^2 as [20]

$$m^2(L) = m^2(\infty) + kL^{-1}. \tag{4}$$

In Fig. 2 we show results for m^2 at a strong-bond concentration $p = 1/4$ for system sizes $L = 4$, 6, 8, 10, and various values of the disorder strength Δ. An approximately linear dependence on $1/L$ is seen for $\Delta < 0.8$. We therefore fit straight lines to those points and extrapolate to obtain the sublattice magnetization for the infinite systems. For $\Delta = 0$ we obtain $m = 0.276 \pm 0.004$ [21]. For $\Delta = 0.70$ the extrapolated m^2 is zero within statistical errors, and this should therefore be close to the critical disorder strength for $p = 1/4$. For $\Delta > \Delta_c$ the scaling with system size must change to $(1/L)^2$ for large L, as $S(\pi, \pi)$ saturates. We have also performed simulations at $p = 1/8$ and $p = 1/2$, and obtained $\Delta_c \approx 0.75$ and $\Delta_c \approx 0.80$, respectively. These points are shown as the solid circles in Fig. 1. The result for $\Delta_c(p = 1/2)$ indicates that the critical concentration p_{c2} as $\Delta \to 1$ is larger than the percolation threshold [16].

For a given p, with $p_{c1} < p < p_{c2}$, as $\Delta \to \Delta_c$ the spatial correlation length ξ_r diverges as $\delta^{-\nu}$, where $\delta = |\Delta - \Delta_c|$. The correlation length in imaginary time ξ_τ diverges as $\delta^{-z\nu}$, where z is the dynamic exponent [22]. With $\Delta > 0$ Lorentz invariance is broken, and one expects $z \neq 1$. The dynamic exponent can be determined by comparing the size dependence of the staggered structure factor $S(\pi, \pi)$ and the staggered susceptibility $\chi(\pi, \pi)$. For a zero-temperature quantum phase transition the exponent η for the algebraic decay of the spatial correlation function $C(r)$ is defined by [15]

$$C(r) \to \frac{1}{r^{D+z-2+\eta}}, \qquad r \to \infty, \tag{5}$$

where D is the spatial dimensionality. The staggered structure factor therefore diverges as $\delta^{-\nu(2-z-\eta)}$. The staggered susceptibility is given by

$$\chi(\pi, \pi) = \frac{1}{L^2} \sum_{j,k} e^{i\vec{\pi}\cdot(\vec{r}_j - \vec{r}_k)} \int_0^\beta d\tau \langle S_j^z(\tau) S_k^z(0) \rangle , \tag{6}$$

and diverges as $\delta^{-\nu(2-\eta)}$. Finite-size scaling theory [23] gives the size dependence of $S(\pi, \pi)$ and $\chi(\pi, \pi)$ at the critical point:

$$S(\pi, \pi) \sim L^{2-z-\eta}, \tag{7a}$$

$$\chi(\pi, \pi) \sim L^{2-\eta}. \tag{7b}$$

Hence, if $S(\pi, \pi) \sim L^{\gamma_S}$ and $\chi(\pi, \pi) \sim L^{\gamma_\chi}$, the dynamic exponent is given by $z = \gamma_\chi - \gamma_S$. In Fig. 3, $\ln[S(\pi, \pi)]$ and $\ln[\chi(\pi, \pi)]$ are graphed versus $\ln(L)$ for two points which we estimate to be close to the phase boundary in the (p, Δ) plane. Least-squares fits of straight lines

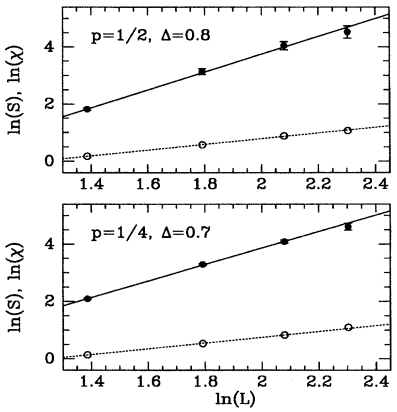

FIG. 3. Finite-size scaling of the staggered structure factor (open circles) and the staggered susceptibility (solid circles) for $p = 1/2, \Delta = 0.8$ (top) and $p = 1/4, \Delta = 0.7$ (bottom). The straight lines are least-squares fits to the points.

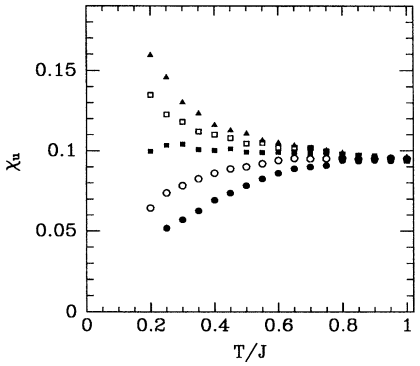

FIG. 4. The uniform spin susceptibility versus temperature for systems of size 32×32 at a strong-bond concentration $p = 1/2$. Solid circles are for $\Delta = 0$, open circles for $\Delta = 0.5$, solid squares for $\Delta = 0.7$, open squares for $\Delta = 0.8$, and solid triangles for $\Delta = 0.9$.

give the slopes $\gamma_s = 1.01 \pm 0.01$, $\gamma_\chi = 2.88 \pm 0.09$ for $p = 1/4, \Delta = 0.7$ and $\gamma_s = 1.00 \pm 0.02$, $\gamma_\chi = 3.12 \pm 0.15$ for $p = 1/2, \Delta = 0.8$. Hence, we have two independent estimates for the dynamic exponent: $z = 1.87 \pm 0.10$ and $z = 2.12 \pm 0.15$. The indicated errors are the statistical errors of the line fits. We have estimated the errors associated with the uncertainty in the determinations of the critical points to be smaller than these errors. For dirty bosons, the hyperscaling theory of Fisher *et al.* gives $z = D$ [15]. The spin model considered here can be mapped onto a hard-core bose system with particle-hole and SU(2) symmetries. The additional symmetries might in principle change the universality class from one of the systems considered in Ref. [15]. Our results for the dynamic exponent are, however, consistent with $z = 2 = D$. The controversy regarding inconsistencies with the exponent obtained in numerical simulations of interacting bosons in a random potential [24] also appears to have been settled recently [25], in favor of the hyperscaling theory.

The value of z has consequences for the behavior of the uniform susceptibility χ_u, which at the transition point is predicted to scale as [15]

$$\chi_u = \frac{\beta}{N} \sum_{i,j} \langle S_i^z S_j^z \rangle \sim \delta^{\nu(D-z)}. \tag{8}$$

Hence, depending on z, the uniform susceptibility diverges, remains finite, or vanishes at the critical point. We have calculated χ_u for $L = 32$ systems at temperatures $T/J = 0.2$–1.0. Results for $p = 1/2$ and various Δ are displayed in Fig. 4. The disorder clearly enhances the low-temperature susceptibility. In view of the fact that χ_u is nonzero at $T = 0$ for the clean 2D Heisenberg model, it is unlikely that the susceptibility of the random systems vanishes as $T \to 0$. According to Eq. (8), this implies that $z \geq 2$, consistent with the above estimates from finite-size scaling. If $z = 2$, χ_u at $\Delta = \Delta_c$ approaches a constant as $T \to 0$, and there is no divergence in this quantity at the order-disorder transition. In 1D, random exchange leads to a low-temperature divergence of the uniform susceptibility [11]. This is also predicted in higher dimensions for systems with longer-range interactions [12]. The natural interpretation of this behavior is that some of the spins are effectively isolated from the rest of the system due to their weak coupling to surrounding strongly coupled spins. One would expect this behavior for the model considered here as well, but only inside the disordered phase, a finite distance away from the order-disorder transition phase boundary, if indeed $z = 2$. It would clearly be interesting to verify this scenario explicitly by studying χ_u at lower temperatures, but unfortunately the computational effort needed exceeds what is presently feasible.

A nonzero $T = 0$ uniform susceptibility implies that the disordered phase is gapless. In order to further investigate the spectrum, we have calculated the imaginary-time correlation function $C(\tau) = (1/N)\sum_i \langle S_i^z(\tau) S_i^z(0) \rangle$ and used the maximum entropy analytic continuation procedure [26] to obtain the real-time wave-vector integrated dynamic structure factor $S(\omega) = (1/N)\sum_q S(q, \omega)$. We have calculated $S(\omega)$ for both clean and random systems. In addition, in order to test the method, we have studied the case where the strong bonds are arranged in a regular staggered pattern such that every spin belongs to a pair connected by a strong bond ($p = 1/4$). In this case one expects a gap for Δ larger than a critical value $\Delta_c \approx 0.39$ [5]. Figure 5 shows low-temperature results for $L = 10$ systems. For the staggered and random cases $\Delta = 0.8$, and the ground states of the corresponding infinite systems are disordered. The staggered system exhibits a clear gap: $S(\omega)$ is a narrow peak centered at $\omega/J \approx 1 + \Delta$, corresponding to the energy required for a singlet-triplet excitation of a spin pair connected by a strong bond. For the clean system there is a broad

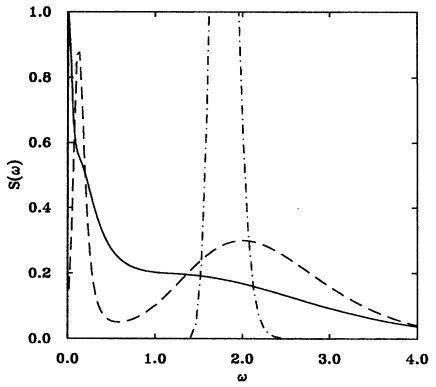

FIG. 5. Wave-vector integrated dynamic structure factors for $L = 10$. The dashed curve is for a clean system at $\beta = 32$, the solid curve for a random system with $p = 1/4$, $\Delta = 0.8$ at $\beta = 64$, and the dash-dotted curve for a staggered strong-bond pattern with $\Delta = 0.8$.

maximum around $\omega/J \approx 2$, and a narrow peak close to $\omega = 0$. In the thermodynamic limit, long wavelength fluctuations of the order parameter lead to a δ-function peak at $\omega = 0$. This peak is shifted here to a nonzero energy by the small gap present in the finite system. For the random case the peak at $\omega = 0$ is due to localized, gapless excitations. There is also more weight at low energies than for the clean system, which we associate with localized excitations involving primarily the weak bonds.

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[1] For a review, see e.g., E. Manousakis, Rev. Mod. Phys. **63**, 1 (1991).

[2] J.D. Reger and A.P. Young, Phys. Rev. B **37**, 5987 (1988); M. Gross *et al.,* Phys. Rev. B **39**, 2484 (1989); K. Runge, Phys. Rev. B **45**, 7229 (1992); U.J. Wiese and H.P. Ying, Z. Phys. B **93**, 147 (1994).

[3] P.W. Anderson, Phys. Rev. **86**, 694 (1952); T. Oguchi, *ibid.* **117**, 117 (1960).

[4] S. Chakravarty, B.I. Halperin, and D.R. Nelson, Phys. Rev. Lett. **60**, 1057 (1988); Phys. Rev. B **39**, 2344 (1989).

[5] R.R.P. Singh *et al.,* Phys. Rev. Lett. **61**, 2484 (1988).

[6] F.D.M. Haldane, Phys. Lett. **93A**, 464 (1983); Phys. Rev. Lett. **50**, 1153 (1983).

[7] S. Sachdev and J. Ye, Phys. Rev. Lett. **69**, 2411 (1992); A. Chubukov and S. Sachdev, Phys. Rev. Lett. **71**, 169 (1993).

[8] M.S. Makivić and H.Q. Ding, Phys. Rev. B **43**, 3562 (1991).

[9] A.W. Sandvik and D.J. Scalapino, Phys. Rev. Lett. **72**, 2777 (1994).

[10] T. Imai *et al.,* Phys. Rev. Lett. **70**, 1002 (1993); **71**, 1254 (1993).

[11] S.K. Ma, C. Dasgupta, and C.K. Hu, Phys. Rev. Lett. **43**, 1434 (1979); D.S. Fisher, Phys. Rev. B **50**, 3799 (1994).

[12] R.N. Bhatt and P.A. Lee, Phys. Rev. Lett. **48**, 344 (1982); S. Sachdev and J. Ye, *ibid.* **70**, 3339 (1993).

[13] M. Guo, R.N. Bhatt, and D. Huse, Phys. Rev. Lett. **72**, 4137 (1994); H. Rieger and A.P. Young, *ibid.* **72**, 4141 (1994).

[14] J. Behre and S. Miyashita, J. Phys. A **25**, 4745 (1992); E. Manousakis, Phys. Rev. B **45**, 7570 (1992).

[15] M.P.A. Fisher *et al.,* Phys. Rev. B **40**, 546 (1989).

[16] Exactly at $\Delta = 1$ the system cannot be ordered for p smaller than the percolation threshold $p_p = \frac{1}{2}$. Quantum fluctuations may destroy the long-range order even for $p > p_p$. One would expect the critical probability $p_{c2}(\Delta \to 1)$ to coincide with the critical value of p at $\Delta = 1$.

[17] A.W. Sandvik and J. Kurkijärvi, Phys. Rev. B **43**, 5950 (1991); A.W. Sandvik, J. Phys. A **25**, 3667 (1992).

[18] In this approach there are no $\Delta\tau$ errors of the type present in world-line methods; J.E. Hirsch *et al.,* Phys. Rev. B **26**, 5033 (1982).

[19] E.H. Lieb and D.C. Mattis, J. Math. Phys. **3**, 749 (1962).

[20] D.A. Huse, Phys. Rev. B **37**, 2380 (1988).

[21] This value is slightly lower than the spin-wave result $m = 0.303$. Our values of m^2 for $L = 4-10$ agree well with Runge's Green's function Monte Carlo results (Ref. [2]). In that work a quadratic term in the fit was included, and a slightly larger extrapolated magnetization was obtained.

[22] J.A. Hertz, Phys. Rev. B **14**, 1165 (1976).

[23] See, e.g., M.N. Barber, in *Phase Transitions and Critical Phenomena,* edited by C. Domb and J. Lebowitz (Academic, London, 1983), Vol. 8.

[24] M. Makivić, N. Trivedi, and S. Ullah, Phys. Rev. Lett. **71**, 2307 (1993).

[25] S. Zhang, N. Kawashima, and J.E. Gubernatis (unpublished).

[26] R.N. Silver, D.S. Sivia, and J.E. Gubernatis, Phys. Rev. B **41**, 2380 (1990); J.E. Gubernatis *et al., ibid.* **44**, 6011 (1991).