4-15-1991

The Dilute Quantum Heisenberg Antiferromagnet

C. C. Wan
University of Pennsylvania

A. Brooks Harris
University of Pennsylvania, harris@sas.upenn.edu

Joan Adler

Recommended Citation
Wan, C., Harris, A., & Adler, J. (1991). The Dilute Quantum Heisenberg Antiferromagnet. *Journal of Applied Physics, 69* (8), 5191-5193. http://dx.doi.org/10.1063/1.348123

The Dilute Quantum Heisenberg Antiferromagnet

Abstract
Series expansions are used to treat the randomly diluted spin-1/2 Heisenberg antiferromagnet at zero temperature. A series is obtained at zero temperature in powers of the concentration for many correlation functions and for the correlation length from which static, dynamic, and crossover exponents are estimated. The correlation length exponent is found to be 0.77±0.10 in two dimensions. The critical concentration for the appearance of long-range order is indistinguishable from the percolation threshold.

Disciplines
Physics | Quantum Physics

The dilute quantum Heisenberg antiferromagnet

C. C. Wan and A. B. Harris
Department of Physics, University of Pennsylvania, Philadelphia, Pennsylvania 19104

Joan Adler[a)]
Department of Physics, Technion, Haifa 32000, Israel

Series expansions are used to treat the randomly diluted spin-$\frac{1}{2}$ Heisenberg antiferromagnet at zero temperature. A series is obtained at zero temperature in powers of the concentration for many correlation functions and for the correlation length from which static, dynamic, and crossover exponents are estimated. The correlation length exponent is found to be 0.77 ± 0.10 in two dimensions. The critical concentration for the appearance of long-range order is indistinguishable from the percolation threshold.

Series expansions have often been useful in determining numerical values of critical exponents, especially in cases where existing theories have been unable to elucidate the nature of the critical phenomena. Here we pursue a program to obtain numerical data on the zero-temperature transition that occurs as a function of concentration p for the spin-$\frac{1}{2}$ Heisenberg antiferromagnet in the presence of quenched random dilution. The Hamiltonian for this system is

$$\mathcal{H}=J \sum_{\langle i,j \rangle} \epsilon_{ij} \mathbf{S}_i \cdot \mathbf{S}_j, \tag{1}$$

where $\mathbf{S}$ is a quantum spin $\frac{1}{2}$, $\langle i,j \rangle$ indicates that the sum is over pairs of nearest neighbors on a d-dimensional hypercubic lattice, and ϵ_{ij} is a random variable which assumes the value unity with probability p if the bond (i,j) is occupied and the value 0 with probability $1-p$ if the bond is unoccupied.

To highlight the differences between the spin-$\frac{1}{2}$ model and the classical model (viz., for the $S \to \infty$ limit), let us note the behavior of the staggered structure factor $C(p)$, which is defined to be

$$C(p)=N^{-1} \sum_{i,j} [\langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle]_{\mathrm{av}} e^{i\mathbf{k}\cdot\mathbf{r}}, \tag{2}$$

where N is the total number of sites in the system, $[\,]_{\mathrm{av}}$ indicates an average over all configurations (of the ϵ_{ij}'s), $\langle\,\rangle$ denotes a zero-temperature average over all state(s) of the ground manifold, and $\mathbf{k}$ is the wave vector associated with the antiferromagnetic order. For a classical system a local "gauge" transformation in which one reverses the sign of $\mathbf{S}_i$ on one sublattice converts $C(p)$ into the zero-wave-vector correlation function for a dilute ferromagnet. Then all spins are parallel in the ground states and $C(p)$ reduces to the mean-square size of connected clusters, which is the percolation susceptibility.[1] Thus for a classical system the threshold concentration at which long-range order sets in coincides with the percolation threshold. One may define a critical exponent associated with $C(p)$ via

$$C(p) \sim |\Delta p|^{-\gamma}, \tag{3}$$

where $\Delta p = p_c - p$ and the critical exponents reduce to that of percolation. For the dilute quantum system $\Delta p = p_Q - p$, where p_Q is the threshold concentration for the appearance of long-range order ($p_Q \geqslant p_c$) and γ is not expected to be identical to the percolation value.

We can similarly define other critical exponents. For instance, if we consider small nonzero temperature, T then we may introduce a crossover exponent[1,2] ϕ by writing

$$C(p,T) \sim |\Delta p|^{-\gamma} f(T/|\Delta p|^{\phi}). \tag{4}$$

Also we may define the correlation length ξ and its associated exponent ν by

$$\xi^{2k} \equiv \sum_{i,j} r_{ij}^{2k} [\langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle]_{\mathrm{av}} e^{i\mathbf{k}\cdot\mathbf{r}} / \sum_{i,j} [\langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle]_{\mathrm{av}} e^{i\mathbf{k}\cdot\mathbf{r}} \tag{5a}$$

$$\sim |\Delta p|^{-2k\nu}, \tag{5b}$$

which we implemented for $k=1$ and $k=2$. For such a zero-temperature transition one expects[3]

$$\gamma=(1-\eta)\nu, \tag{6}$$

where η is defined by $|[\langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle]_{\mathrm{av}}| \sim r_{ij}^{1-d-\eta}$. The difference between Eq. (6) and the usual formula, $\gamma=(2-\eta)\nu$, is due to the additional time dimension used to describe zero-temperature quantum systems.[4] Likewise, we write the singular part of the configurationally averaged ground-state energy $E(p)$ as

$$E(p)=|\Delta p|^{1-\alpha}, \tag{7}$$

with[3] $\alpha=2-(d+z)\nu$, where z, the so-called dynamic exponent, is defined so that the characteristic energy scale is of order $\xi^{-z\nu}$. The staggered susceptibility χ_s, which is defined to have the dimensions of (energy)$^{-1}$, consists of two types of terms:[5]

$$\chi_s=(A/T)+(B/J), \tag{8}$$

where

$$A=\left[\sum_{\alpha} \langle \mathbf{S}_\alpha(\mathbf{k}) \mathcal{P} \mathbf{S}_\alpha(-\mathbf{k}) \rangle \right]_{\mathrm{av}}, \tag{9a}$$

$$\frac{B}{J}=2\left[\sum_{\alpha} \langle \mathbf{S}_\alpha(\mathbf{k}) (\mathcal{I}-\mathcal{P}) (\mathcal{H}-E_0\mathcal{I})^{-1} \mathbf{S}_\alpha (-\mathbf{k}) \rangle \right]_{\mathrm{av}}, \tag{9b}$$

[a)] Also at: School of Physics and Astronomy, Tel Aviv University, Tel Aviv 69978, Israel.

 0021-8979/91/085191-03$03.00

where α labels Cartesian components, $\mathscr{I}$ is the unit operator, and $\mathscr{P}$ is a projection operator that is unity only in the ground manifold whose energy is E_0. Finally, we consider the fourth-order staggered susceptibility. It is given by more complicated expressions than Eqs. (8) and (9), so we confine our attention to its zero-temperature limit and write

$$\chi_{s,4} \equiv \lim_{T\to 0} T^2 \frac{\partial^4 F}{\partial h_s^4}, \tag{10}$$

where h_s is the staggered field. These quantities have the asymptotic behavior

$$B(p) \sim |\Delta p|^{-\gamma - z\nu}, \tag{11a}$$

$$A(p) \sim |\Delta p|^{-\gamma - z\nu + \phi}, \tag{11b}$$

$$\chi_{s,4} \sim |\Delta p|^{-(d\nu + 2\gamma + 3z\nu - 3\phi)}. \tag{11c}$$

The aim is to determine p_Q and the above critical exponents. For this purpose we constructed series expansions of these quantities in powers of p up to order p^{13}. To obtain such an expansion for any quantity X we must calculate X for all possible isolated clusters Γ consisting of up to 13 bonds. In this task we are aided by the Lieb–Mattis theorem[6] which says that for any cluster the total spin S_{tot} of the true ground state is identical to the value of S_z in the Néel state. Also, when $S_{tot} \neq 0$, the sum over the degenerate ground-state manifold can be simplified using the Wigner–Eckart theorem.[7] Then

$$[X]_{av} = \sum_{\Gamma} P(\Gamma) X(\Gamma) = \sum_{\Gamma} p^{n_b(\Gamma)} X_c(\Gamma), \tag{12}$$

where $P(\Gamma)$ is the occurrence probability of the cluster Γ, $n_b(\Gamma)$ is the number of bonds in Γ, and $X_c(\Gamma)$ is the cumulant value of X (which is obtained recursively by subtracting the contributions from cumulants of all subdiagrams of Γ). For quantities that only depend on the topology (and not on the exact shape) of the cluster, the sum over Γ can be restricted to topologically inequivalent diagrams, since we have the weak embedding constants for general hypercubic lattice in d dimensions. (For the series involving the correlation length this simplification could not be made, and those results were confined to $d=2$ and 3.) Critical exponents were obtained from the series by Padé analyses or more general methods as described previously.[8] For instance, for $d=2$ the the coefficients in the series for the correlation correlation length, starting with the constant term and going up to order p^{11}, are 0.0000, 1.0000, 0.6667, 14.7718, −28.9345, 396.6181, −2507.5602, 21 322.9721, −163 559.2768, 1 276 223.5022, −9 657 938.4516, and 71 906 968.9306. From the original series, we can obtain further series either by dividing one series by another or by term by term division of two series. The latter procedure[9] has the advantage that it yields a series whose divergence occurs at the known value $p=1$ in contrast to the former series whose threshold remains at the unknown value p_Q.

In principle, the first question should be to determine p_Q, and in particular to see whether $p_Q = p_c$. To answer this question we show in Fig. 1 the phase diagram we expect for this system. There we incorporate the result of Chakravarty, Halperin, and Nelson[10] that there is a critical value for the coupling constant in the pure system for the nonlinear sigma model. Also it seems certain that the condition for randomness to be relevant,[3] viz., $\alpha + \nu > 0$, holds so that the pure system fixed point is unstable to dilution. Since we believe quantum randomness and classical randomness are in different universality classes, we assume the percolation fixed point to be unstable in the g direction. Therefore there is a critical surface, whose projection in the g-p plane we show in Fig. 1, that surrounds the Néel ordered phase. The quantum random fixed point does not lie in the p-g plane because it requires a nontrivial fixed distribution of coupling constants. This picture indicates that the critical concentration should in fact depend on $1/S$. However, our series were not long enough and well enough behaved to detect a nonzero value of $\delta p \equiv p_Q - p_c$.

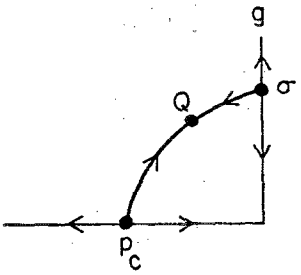

FIG. 1. Fixed-point structure of the randomly dilute quantum antiferromagnet in the p-g plane, where g is the coupling constant in the nonlinear sigma model. At the dilute quantum fixed point Q, a fixed distribution of coupling of finite width (i.e., inequivalent to a pure system) is maintained. This point, although on the critical surface, does not lie in the p-g plane.

It might be possible to show that $\delta p \neq 0$ by considering the high-dimensionality limit. Although we expect Δp to decrease with increasing dimension,[11] the high-dimensionality limit is often quite simple for classical models, because there loopless, or tree, clusters dominate. In fact, for most classical models the two-point correlation function for high d is given in terms of chain diagrams. The case of lattice animals is a notable exception in which loopless diagrams with all numbers of free ends are important[12] in high d. In the present case we find that in the high-dimensionality limit our series have important contributions from all loopless diagrams. In fact, most of our series alternate in sign, indicating the importance of an unphysical singularity at small negative p. Similar behavior was found previously[13] for quantum percolation. For example, in the limit of high dimension the series for $C(p)$ becomes a power series in the variable dp with coefficients, starting with the constant term, which are 0.2500, 0.5000, −0.3333, 1.7299, −4.6647, 23.1059, −115.3064, 664.3666, −3935.6508, 23 961.6815, −147 319.3240, 912 274.4025, −5 675 735.2061, and 35 459 841.9534. To summarize: Quantum fluctuations, like lattice animals, have interesting behavior in high dimension.

Finally, we discuss the numerical values we found for the critical exponents. Since our analyses were not very sensitive to the exact choice of p_Q, we set $p_Q = p_c$. In most cases the results given in Table I represent several independent methods of analysis and the error bars reflect the degree of consistency between different methods. The series for $E(p)$ could not be analyzed, as is often the case for

TABLE I. Critical exponents for quantum dilution.

	$d=2$	$d=3$	$d=8$
ν	0.77 ± 0.1	0.575 ± 0.05	⋯
$z\nu$	1.30 ± 0.1	1.30 ± 0.1	1.33 ± 0.03
ϕ	1.6 ± 0.3	⋯	1.5 ± 0.05
$\phi - z\nu$[a]	0.25 ± 0.2	0.25 ± 0.2	0.10 ± 0.1
γ	0.70 ± 0.1	0.35 ± 0.1	0.19 ± 0.01

[a]The entries for $\phi - z\nu$ are values obtained from the series $A(p)/C(p)$.

specific-heat series. For $d=2$ and 3 we used several of the above series including those for ξ^2 and ξ^4 to get estimates for the correlation length exponent ν. The other exponents could then be determined from the series of Eq. (11). We expected to find $\phi=z\nu$ because $z\nu$ is the exponent associated with the time axis and ϕ is associated with the equivalent temperature axis. However, as can be seen from Table I, we did not quite get this result. Perhaps this is an indication of the reliability of our results. The unusually small values of γ are a consequence of Eq. (6), which is a unique reflection of quantum critical phenomena. Perhaps the most important result in Table I is that ν is very definitely much less than for percolation, where $\nu=\frac{4}{3}$ in $d=2$. The fact that ν is different from its percolation value proves that the quantum antiferromagnet at percolation is not described at the percolation fixed point as the classical system is.[1,2] Or in other words, at the percolation fixed point $1/S$ is relevant. Although ν is not too different from the nonlinear sigma model result,[10] ($\nu\approx0.7$), our value of z that is greater than unity indicates that the nonlinear sigma model fixed point is indeed unstable to randomness. So although we have not shown that δp is nonzero, our results are otherwise consistent with Fig. 1. It is obvious that there is much to be understood, although our results are the first to indicate rough values for the critical exponents of this quantum dilution fixed point.

This work was supported in part by the National Science Foundation (NSF) under Grant No. DMR-88-15469 and by a grant from the U.S.-Israel Binational Science Foundation. One of us (J. A.) acknowledges the support of the Israel Academy of Science. We thank B. I. Halperin and T. C. Lubensky for helpful discussions concerning scaling relations. We thank A. Aharony for helpful suggestions. We thank R. Fisch for some helpful comments on the location of p_Q. The computations were done on a Stardent Titan 3000 computer supported by the NSF MRL program under Grant No. DMR-88-19885.

[1] M. J. Stephen and G. S. Grest, Phys. Rev. Lett. **38**, 567 (1977).
[2] A. B. Harris and T. C. Lubensky, Phys. Rev. B **35**, 6964 (1987).
[3] D. Boyanovsky and J. Cardy, Phys. Rev. **26**, 154 (1982); D. Boyanovsky and J. Cardy, Phys. Rev. **27**, 6971 (1983).
[4] J. Hertz, Phys. Rev. B **14**, 1165 (1976).
[5] J. H. Van Vleck, *Theory of Electric and Magnetic Susceptibilities* (Oxford University Press, Oxford, 1927).
[6] E. H. Lieb and D. C. Mattis, Ann. Phys. (NY) **16**, 407 (1961); E. H. Lieb and D. C. Mattis, J. Math. Phys. **3**, 749 (1962).
[7] See M. E. Rose, *Elementary Theory of Angular Momentum* (Wiley, New York, 1957), p. 85.
[8] L. Klein, J. Adler, A. Aharony, A. B. Harris, and Y. Meir, Phys. Rev. B **40**, 4824 (1989).
[9] D. L. Hunter and G. A. Baker, Jr., Phys. Rev. B **7**, 3346 (1973); Y. Meir, J. Phys. A **20**, L349 (1987).
[10] S. Chakravarty, B. I. Halperin, and D. R. Nelson, Phys. Rev. **39**, 2344 (1989).
[11] R. Raghavan and D. C. Mattis, Phys. Rev. B **23**, 4791 (1981); Y. Shapir, A. Aharony, and A. B. Harris, Phys. Rev. Lett. **49**, 486 (1982).
[12] A. B. Harris, Phys. Rev. B **26**, 337 (1982).
[13] A. B. Harris, Phys. Rev. B **29**, 2519 (1984), and Appendix A therein.