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Critical Exponents of the Quantum Phase Transition in a Planar Antiferromagnet

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We have performed a large scale quantum Monte Carlo study of the quantum phase transition in a planar spin-1/2 Heisenberg antiferromagnet with CaV_4O_9 structure. We obtain a dynamical exponent $z = 1.018 \pm 0.02$, consistent with Lorentz invariance. The critical exponents β, ν and η agree within our errors with the classical 3D $O(3)$ exponents, expected from mapping to the nonlinear sigma model.

KEYWORDS: quantum phase transition, quantum Heisenberg antiferromagnet, quantum critical, renormalized classical, quantum disordered, non-linear sigma model, Berry phase, quantum Monte Carlo, critical exponent

Instead of classical transitions controlled by temperature T, a quantum phase transition between a symmetry broken phase with long-range Néel order and a quantum disordered state with a finite spin excitation gap, may be realized at $T = 0$ by controlling a parameter g to increase quantum fluctuations. Criticalities around such quantum phase transitions at $g = g_c$ may reflect inherent quantum dynamics of the system and yield unusual universality classes with rich physical phenomena.[1)] In this letter we discuss a two-dimensional quantum Heisenberg antiferromagnet (2D QAFM) that exhibits such a quantum phase transition.

The critical behavior of classical spin systems near a finite temperature phase transition and the critical exponents have been calculated with high accuracy using cluster Monte Carlo methods.[7)] For quantum phase transitions in quantum spin systems, however, only a few preliminary calculations on small lattices have been possible. The recent development of cluster algorithms for quantum Monte Carlo (QMC) simulations[2,3)] has made it feasible to perform high precision simulations also for quantum phase transitions. Combining quantum Monte Carlo results on lattices of up to 20 000 spins with the exact finite size scaling results of Hasenfratz and Niedermayer[4)] we can, for the first time, calculate all the critical exponents of the quantum phase transition in a planar antiferromagnet with good accuracy.

Approaching the quantum critical point from the disordered side, the spatial correlation length diverges with the correlation length exponent ν. The space and time dimensions are not necessarily equivalent, and the correlation length in the time direction diverges, in general, with a different exponent $z\nu$, where z is the dynamical exponent. Related to the divergence of the correlation length is a vanishing of the spin excitation gap with the same exponent $z\nu$. When passing through the critical point long-range order is established. The order parameter in the case of a Néel ordered antiferromagnet is the staggered magnetization m_s. Near the critical point, m_s vanishes with the order parameter exponent β. At the critical point itself the real space staggered spin correlation shows a power-law falloff with power $2 - d - z - \eta$, where η is the correlation exponent. These four exponents are related by the usual scaling law

$$2\beta = (d + z - 2 + \eta)\nu, \tag{1}$$

where the effective dimension is $d + z$ in a quantum system.

Quantum critical behavior of a planar antiferromagnet has been intensively studied by a number of groups. Most analytic calculations are based on the $O(3)$ nonlinear sigma model (QNLσM), which exhibits a quantum phase transition as the coupling strength g is varied. For $g < g_c$, the ground state shows long range $O(3)$ order, while for $g > g_c$ it is quantum disordered.

The critical exponents of the QNLσM can be determined from simple symmetry, universality and scaling arguments.[5,6)] As the QNLσM is Lorentz invariant the correlation length is, up to scale factors, the same in the space and time directions. Consequently the correlation length exponent in the spatial directions ν and in the time direction $z\nu$ are the same, hence $z = 1$.

Furthermore, the 2D $O(3)$ QNLσM is equivalent to the 3D classical $O(3)$ sigma model. This, in turn, is in the universality class of the classical 3D Heisenberg ferromagnet. The exponents β, ν and η should thus be the same as the well-known classical exponents of this model (see Table I).

Chakravarty, Halperin and Nelson[5)] discussed the phase diagram of a planar Heisenberg antiferromagnet using the QNLσM. They concentrated on the ordered phase and described it as a classical 2D antiferromagnet with renormalized parameters.

Chubukov, Sachdev and Ye[6)] investigated in detail the quantum critical regime of the QNLσM. They made further predictions based on scaling arguments. The spin stiffness ρ_s is the coefficient of the quadratic dependence of the ground state energy on a twist in the spatial

Table I. Critical exponents β, ν, η and z. Listed are the estimates of the exponents without making any assumption for z, and the best estimate if Lorentz invariance ($z = 1$) is assumed. For comparison the exponents of the 3D classical Heisenberg (O(3)) model, the 3D Ising model and the 2D quantum mean field exponents are listed. The errors given include the uncertainties in the critical point.

model	ν	β	η	z
2D QAFM	0.685 ± 0.035	0.345 ± 0.025	0.015 ± 0.020	1.018 ± 0.02
Lorentz invariant 2D QAFM	0.695 ± 0.030	0.345 ± 0.025	0.033 ± 0.005	1 (assumption)
bilayer QAFM[13]			0.03 ± 0.01	1.08 ± 0.05
3D O(3)[7]	0.7048 ± 0.0030	0.3639 ± 0.0035	0.034 ± 0.005	—
3D Ising[8]	0.6294 ± 0.0002	0.326 ± 0.004	0.0327 ± 0.003	—
mean field	1	1/2	0	1

boundary conditions (similar to the Drude weight in itinerant fermionic models). On the ordered side it vanishes as

$$\rho_s \propto (g_c - g)^{(d+z-2)\nu} = (g_c - g)^{\nu}, \qquad (2)$$

where the second equivalence comes from the prediction that $z = 1$. The spin wave velocity c scales as

$$c \propto (g - g_c)^{\nu(z-1)} \qquad (3)$$

and is thus regular at the critical point if $z = 1$. The zero temperature uniform susceptibility can be expressed through the spin stiffness as $\chi_u(T = 0) = 2\rho_s/3(\hbar c)^2$. At the critical point the temperature dependence of the uniform susceptibility is universal:

$$\chi_u = \Omega_1(\infty)\left(\frac{g\mu_B}{\hbar c}\right)^2 T, \qquad (4)$$

where $\Omega_1(\infty)$ is a universal constant. Estimates for $\Omega_1(\infty)$ are listed in Table II.

The equivalence of the 2D QAFM to the 2D QNLσM is still in question, because of the existence of the Berry phase terms in the QAFM that are not present in the QNLσM.[9] These Berry phase terms are non-local phase terms and play a decisive role as the topological term in one-dimensional spin chains. Because of this topological term spin chains with half integer spin have gapless ground states while integer spin chains exhibit a spin gap.[10]

The role of the Berry phase terms in two dimensions however is unclear. It has been argued that these terms cancel in special cases, such as in the bilayer model.[11,12] In this case it is plausible that the quantum phase transition is in the same universality class as the QNLσM. This was confirmed by quantum Monte Carlo calculations by Sandvik *et al.*[11,13,14] They investigated the bilayer QAFM on lattices with up to $10 \times 10 \times 2$ spins. Although these lattices are quite small they still found an agreement of the exponents z and η with the QNLσM predictions.[11,13] (see Table I). In the absence of Berry phase terms the proposed equivalence of the QAFM and the QNLσM is supported by these simulation results.

In general these Berry phase terms exist however. Chakravarty *et al.* argue, that they can change the critical behavior, leading to different exponents.[5,15] Chubukov *et al.*, on the other hand, argued that the Berry phase terms are dangerously irrelevant, that is, irrelevant at the critical fixed point separating the two phases, but relevant in the quantum disordered phase.[6,17]

Table II. Universal prefactor $\Omega_1(\infty)$ in the linear temperature dependence of the uniform susceptibility at criticality. Listed are the results for the quantum nonlinear sigma model in a $1/N$ expansion, the results by classical Monte Carlo simulation on a 3D classical rotor model and the result of this study.

method	Ref.	$\Omega_1(\infty)$
1/N expansion	ref. 2	0.2718
classical Monte Carlo	ref. 2	0.25 ± 0.04
quantum Monte Carlo	this study	0.26 ± 0.01

Previous numerical simulations on dimerized square lattices[13,18] were not consistent with the QNLσM predictions. This could be an effect of the Berry phase terms that are present in this model. The reliability of the results, however, is questionable because of the restriction to very small lattices of 12×12 spins and because of complications with scaling arising from inequivalent spatial directions.

We performed large-scale quantum Monte Carlo simulations to investigate this question. Using the new quantum cluster algorithms[2,3] we could simulate lattices two orders of magnitude larger and at one order of magnitude lower temperatures and got more accurate and new results.

The universality class of a phase transition does not depend on the microscopic details of the lattice structure, therefore, we are free to choose the best lattice for our purposes. We chose the CaV_4O_9 lattice, a 1/5-th depleted square lattice depicted in Fig. 1, for our calculations. In contrast to the bilayer model, Berry phase terms are present on this lattice.[17] Its advantage over the dimerized square lattice is that both space directions are equivalent. We performed our simulations on square lattices with $N = 8n^2$ spins, where n is an integer. Our largest lattice contained 20 000 spins. For the following discussion it is helpful to introduce the linear system size L in units of the bond lengths a of the original square lattice: $L \equiv a\sqrt{5N/4}$.

The phase diagram of this lattice has been discussed in detail.[19] By removing every fifth spin we obtain a lattice consisting of four-spin plaquettes linked with dimer bonds. We label the couplings in a plaquette J_0 and the inter-plaquette couplings J_1. By controlling the ratio of J_1 and J_0, we can tune from Néel order at $J_1 = J_0$ to a

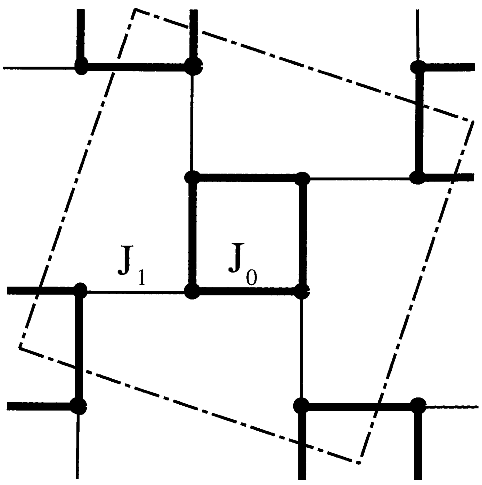

Fig. 1. Lattice structure of the 1/5-th depleted square lattice of CaV_4O_9. The dashed square indicates the eight spin unit cell used in our calculations.

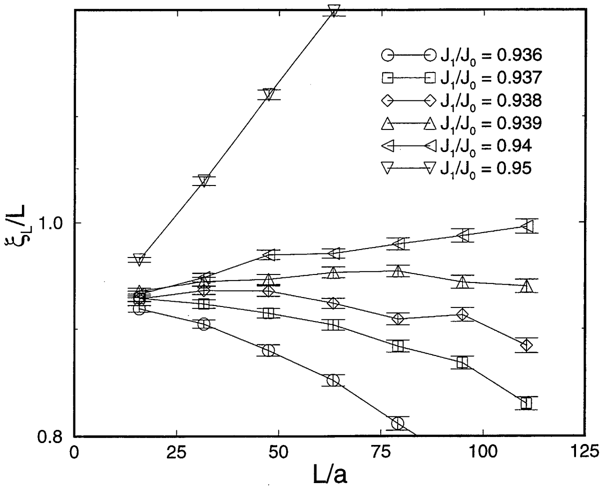

Fig. 2. Plot of the ratio of correlation length divided by system size ξ_L/L. At the critical point the correlation length calculated in a finite system is proportional to the system size. This is the case for $g = J_1/J_0 = 0.939 \pm 0.001$.

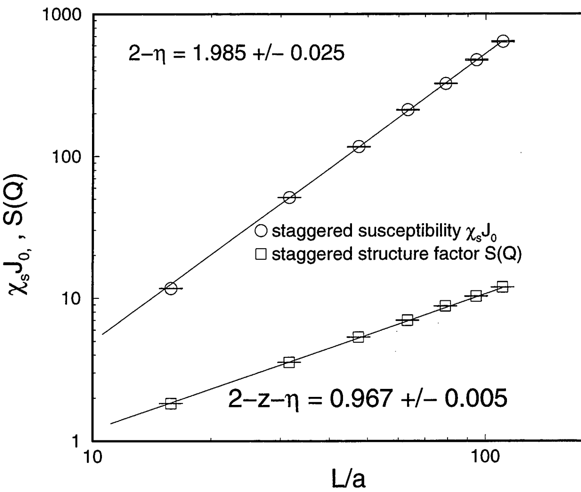

Fig. 3. Finite size scaling of the staggered structure factor and susceptibility at the critical point. The straight lines are fits to the finite size scaling forms eqs. (5) and (6).

quantum disordered "plaquette RVB" ground state with a spin gap $\Delta = J_0$ at $J_1 = 0$. The control parameter g of the quantum phase transition is the coupling ratio J_0/J_1 in this model.

At an intermediate coupling ratio $(J_1/J_0)_c$ the system exhibits a quantum phase transition. The first step in the determination of the critical behavior is a high precision estimate of the critical point g_c. We have calculated the second moment correlation length ξ_L on systems of various sizes L. The temperature was chosen to be $k_B T = J_0 a/L$, keeping the finite 2+1 dimensional system in the cubic regime. From standard finite size scaling arguments it follows that this correlation length ξ_L scales proportional to the system size L at criticality. We calculated the ratio ξ_L/L, shown in Fig. 2, for a variety of couplings and system sizes up to $N = 9600$, and determined the critical coupling to be $(J_1/J_0)_c = 0.939 \pm 0.001$.

Next, we calculated the finite size scaling of both the staggered structure factor $S(\mathbf{Q}) = L^2 m_s$ and of the corresponding staggered susceptibility. At criticality they scale as

$$S(\mathbf{Q}) \propto L^{2-z-\eta} \tag{5}$$

$$\chi_s \propto L^{2-\eta}. \tag{6}$$

The temperature was chosen to be $k_B T = J_0 a/(4L)$. This was low enough to see the ground state properties on the finite lattice. By fitting our results, shown in Fig. 3, we obtained the estimates $z = 1.018 \pm 0.02$ and $\eta = 0.015 \pm 0.020$. This is consistent with the Lorentz invariance ($z = 1$) expected from the mapping to the QNLσM. We will discuss η below with the other exponents. From these fits it is noted that at least $N = 800$ spins are necessary to obtain good scaling.

The remaining exponents β and ν are best calculated from the magnetization m_s and the spin stiffness ρ_s on the ordered side. Good estimates for m_s and ρ_s can be obtained from equations by Hasenfratz and Niedermayer.[4] They calculated the *exact* finite-size and finite-temperature values of the low-temperature uniform and staggered susceptibilities χ_u and χ_s for the ordered phase of a 2D QAFM on a lattice with the symmetries of a square lattice. Their equations, determined by chiral perturbation theory, are correct for the low temperature regime $k_B T \ll 2\pi\rho_s$ with cubic geometry $k_B T L/\hbar c \approx 1$. Up to second order in T (or $1/L$ respectively) the susceptibilities are universal, determined by only three parameters: the staggered magnetization m_s, the spin stiffness ρ_s and the spin wave velocity c. Two high precision quantum Monte Carlo studies have confirmed these equations for the square lattice QAFM.[3,20]

We have calculated the susceptibilities for a wide range of couplings $0.95 < J_1/J_0 < 1.1$, lattice sizes $800 < N < 16200$ and temperatures $0.006 < T/J_0 < 0.1$. The fits to the Hasenfratz-Niedermayer equations are all excellent, with χ^2/d.o.f. ≈ 1.5. This also confirms the universality of the Hasenfratz-Niedermayer equations. From the fits we obtained the staggered magnetization m_s, the spin stiffness ρ_s and the spin wave velocity c. The exponents

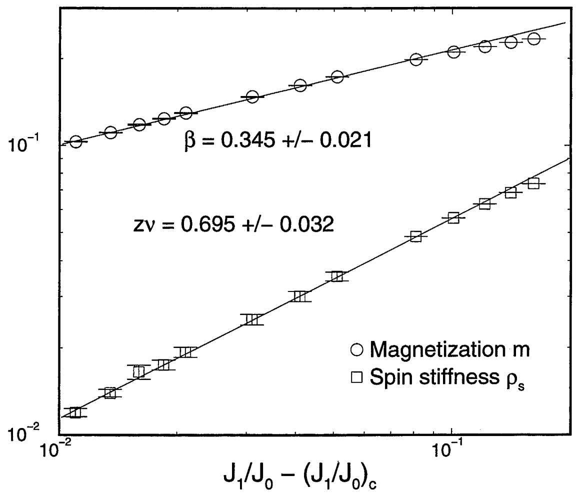

Fig. 4. Staggered magnetization m_s and spin stiffness ρ_s calculated by a fit of low temperature susceptibilities on finite lattices to the Hasenfratz-Niedermayer equations.[4] The straight lines are fits used to obtain the exponents β and ν.

β and ν could then be obtained in a straightforward manner (Fig. 4) and are listed in Table I.

Let us now discuss the results. First, we note that the exponents satisfy the scaling relation eq. (1), confirming the validity of the scaling ansatz for this quantum phase transition. The exponents β, ν and η are in good agreement with the exponents of the 3D classical O(3) or Heisenberg model. They are, however, incompatible with the mean field exponents suggested by Katoh and Imada from their calculations on small lattices.[18]

Assuming Lorentz invariance ($z = 1$) we can improve our estimates for the other exponents. The agreement of the improved estimates with the 3D O(3) exponents becomes even better. We can rule out the mean field universality class.[18] Furtermore we can also reject the Ising universality class with more than 97% confidence (Table I).

This agreement suggests that the Berry phase terms in the 2D QAFM are indeed dangerously irrelevant, as proposed by Chubukov *et al.*[6] To further test their predictions, we calculated the uniform susceptibility close to criticality down to $T = 0.02$, more than an order of magnitude lower than that in ref. 11. We extrapolated the finite size results on lattices with up to $N = 20000$ spins to the thermodynamic limit. Looking for the coupling at which a linear behavior occurs gives an independent estimate of the critical point: $(J_1/J_0)_c = 0.939 \pm 0.002$, in agreement with the above estimate. The linear slope is $\Omega_1(\infty)(J_0/\hbar c)^2 = 0.238 \pm 0.003$. By extrapolating the spin wave velocity determined in the ordered phase by the Hasenfratz-Niedermayer fit to the critical point we obtain $\hbar c/J_0 = 1.04 \pm 0.02$ and thus $\Omega_1(\infty) = 0.26 \pm 0.01$, again in agreement with Chubukov *et al.*[6] (Table II).

To summarize, we have, for the first time, calculated all the critical exponents β, ν, z and η of the quantum critical point in a planar antiferromagnet by a large scale quantum Monte Carlo study. Our exponents agree with predictions made by a mapping to the 2D quantum nonlinear sigma model. The dynamical exponent is $z = 1.018 \pm 0.02$, consistent with Lorentz invariance. The other exponents agree with the 3D classical O(3) exponents.

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