Critical exponents of the quantum phase transition in a planar antiferromagnet

Matthias Troyer, Masatoshi Imada and Kazuo Ueda
Institute for Solid State Physics, University of Tokyo, Roppongi 7-22-1, Tokyo 106, Japan

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$_2$O$_5$ structure. We obtain a dynamical exponent $z = 1.018 \pm 0.02$. The critical exponents $\beta, \nu$ and $\eta$ agree within our errors with the classical 3D $O(3)$ exponents, expected from a mapping to the nonlinear sigma model. This confirms the conjecture of Chubukov, Sachdev and Ye [Phys. Rev. B 49, 11919 (1994)] that the Berry phase terms in the planar Heisenberg antiferromagnet are dangerously irrelevant.

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.

The most prominent example are the high temperature superconductors. There the quantum spin fluctuations are thought to lead to $d$-wave superconductivity as soon as antiferromagnetism is suppressed by hole doping.

In this letter we want to discuss a two dimensional quantum Heisenberg antiferromagnet (2D QAFM) that exhibits such a quantum phase transition. We will present strong numerical support for the conjecture that the 2DQAFM is in the same universality class as the quantum nonlinear sigma model (QNL$\sigma$M) even when Berry phase terms are present.

The universality class is characterized by the critical exponents. Approaching the quantum critical point from the disordered side the spatial correlation length diverges with the correlation length exponent $\nu$. The space and time dimensions are however 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. In a Lorentz invariant system space and time dimensions are equivalent and $z = 1$. 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 $\beta$. At the critical point itself the real space staggered spin correlation shows a power-law falloff with power $2 - d - z - \eta$, where $\eta$ is the correlation exponent. These three exponents are related by the usual scaling law

\[ 2\beta = (d + z - 2 + \eta)\nu, \]

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 QNL$\sigma$M. The critical exponents of the QNL$\sigma$M can be determined from simple symmetry, universality and scaling arguments [4,5]. Lorentz invariance implies that $z = 1$. Furthermore the 2D QNL$\sigma$M is equivalent to the 3D classical sigma model. This in turn is in the universality class of the 3D classical $O(3)$ model, or the classical 3D Heisenberg ferromagnet. The exponents $\beta, \nu$ and $\eta$ should thus be the same as the well known classical exponents of these models (see Tab. I).

Chakravarty, Halperin and Nelson have discussed the phase diagram of a planar Heisenberg antiferromagnet by using the QNL$\sigma$M. In their discussions they concentrate on the ordered phase and describe it as a classical 2D antiferromagnet with renormalized parameters.

Chubukov, Sachdev and Ye have investigated the quantum critical regime of the QNL$\sigma$M in close detail. They make some further predictions based on scaling arguments. On the ordered side the spin stiffness $\rho_s$ vanishes as

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

where the second equivalence comes from the prediction that $z = 1$. They also predict that the uniform susceptibility at the critical point is universal:

\[ \chi_u = \Omega_1(\infty) \left( \frac{\mu_b}{hc} \right)^2 T. \]

Here $c$ is the spin wave velocity and $\Omega_1(\infty)$ a universal constant. Estimates for $\Omega_1(\infty)$ are listed in Tab. II.

The spin wave velocity $c$ scales as

\[ c \propto (g - g_c)^\nu(z - 1) \]

and is thus regular at the critical point if $z = 1$.

The equivalence of the 2D QAFM to the 2D QNL$\sigma$M however is still an open question because of the existence of Berry phase terms in the QAFM that are not present in the QNL$\sigma$M [6]. It has been argued that these terms cancel in special cases, such as in the bilayer model [8]. Then it is plausible that the quantum phase transition is in the same universality class as the QNL$\sigma$M. This
was confirmed by quantum Monte Carlo calculations of Sandvik and coworkers. They have investigated the finite size scaling of the ground state structure factor and susceptibilities on lattices with up to $10 \times 10 \times 2$ spins. Although these lattices are quite small they still found good agreement of the exponents $z$ and $\eta$ with the QNLσM predictions (see Tab. I). In another study Sandvik et al. have investigated finite temperature properties of the bilayer QAFM on larger lattices and also found good agreement with the QNLσM predictions. In the absence of Berry phase terms the equivalence of the QAFM and the QNLσM is quite well established by these simulations.

But in general these Berry phase terms exist. Chakravarty et al. argue that they can change the critical behavior and lead to different exponents. Chubukov et al. on the other hand argue that the Berry phase terms are dangerously irrelevant and do not influence the critical behavior. Previous numerical simulations on dimerized square lattices are indeed not consistent with the QNLσM predictions. The reliability of the results however is questionable because of the restriction to very small lattices of $12 \times 12$ spins and because of complications with scaling arising from inequivalent spatial directions. On the other hand the discrepancy could be an effect of the Berry phase terms that are present in the dimerized square lattice but probably not in the bilayer.

Using the new quantum cluster algorithms we could simulate much larger lattices at lower temperatures. On these larger lattices we find perfect agreement with predictions made based upon the 2D QNLσM despite the presence of Berry phase terms.

As the universality class of a phase transition does not depend on the microscopic details of the lattice structure we are free to choose the best lattice for our purposes. We have chosen the CaV$_4$O$_9$ lattice, a 1/5-th depleted square lattice depicted in Fig. 1 for our calculations. There are three reasons for this choice. Firstly the Berry phase terms are present on this lattice. Next both space directions are equivalent, in contrast to the dimerized square lattice. This makes the scaling analysis easier. Finally at the quantum critical point all the couplings are nearly equal in magnitude, which is also optimal from a numerical point of view. We have performed our simulations on square lattices with $N = 8n^2$ spins, where $n$ is an integer. Our largest lattices contained 20 000 spins. For the following discussion it is useful to introduce the linear system size $L$ in units of the bond lengths $a$ of the original square lattice: $L \equiv \sqrt{5N/4a}$.

The phase diagram of this lattice has been discussed in detail in Ref. [15]. By removing every fifth spin we obtain a lattice consisting of four-spin plaquettes linked by dimer bonds. We label the couplings in a plaquette $J_0$ and the inter-plaquette couplings $J_1$. By controlling the ratio of these couplings $J_1/J_0$ we can tune from Néel order at $J_1 = J_0$ to a quantum disordered “plaquette RVB” ground state with a spin gap $\Delta = J_0$ at $J_1 = 0$.

At some intermediate coupling ratio $(J_1/J_0)_c$ the systems has 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 $\xi_2$ on systems of various sizes $L$. The temperature was chosen to be $k_BT = J_0a/L$, keeping the finite $2 + 1$ dimensional system in the cubic regime. From standard finite size scaling arguments it follows that this correlation length $\xi_L$ scales proportional to the system size $L$ at criticality. We have calculated the ratio $\xi_L/L$ (shown in Fig. 2) for a variety of couplings and system sizes up to $N = 9600$ and have determined the critical coupling to be $(J_1/J_0)_c = 0.939 \pm 0.001$.

Next we have calculated the finite size scaling of both the staggered structure factor $S(Q) = L^2m_s$ and of the corresponding staggered susceptibility. At criticality they scale like

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

$$\chi_s \propto L^{2-\eta}$$

The temperature was chosen to be $k_BT = J_0a/(4L)$. This was low enough to see the ground state properties on the finite lattice. By fitting our results shown in Fig. 3 we obtain the estimates $z = 1.018 \pm 0.02$ and $\eta = 0.015 \pm 0.020$. This is perfectly consistent with the Lorentz invariance ($z = 1$) expected from a mapping to the QNLσM. We will discuss $\eta$ below together with the other exponents. From these fits it is also obvious that at least $N = 800$ spins are necessary to obtain good scaling.

The remaining exponents $\beta$ and $\nu$ are best calculated from the magnetization $m_s$ and the spin stiffness $\rho_s$ on the ordered side. Good estimates for $m_s$ and $\rho_s$ can be obtained from the Hasenfratz-Niedermayer equations [14].

These authors have calculated the exact finite-size and finite-temperature values of the low-temperature uniform and staggered susceptibilities $\chi_u$ and $\chi_s$ 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 $k_BT \ll 2\pi\rho_s$ with cubic geometry $k_BT/Lc \approx 1$. 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 $\rho_s$ and the spin wave velocity $c$. Two high precision quantum Monte Carlo studies have confirmed their equations for the square lattice QAFM.

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 $\chi^2/d.o.f. \approx 1.5$. This is another confirmation...
of the universality of the Hasenfratz-Niedermayer equations. From the fits we obtain the staggered magnetization $m_s$, the spin stiffness $\rho_s$ and the spin wave velocity $c$. The exponents $\beta$ and $\nu$ can then be obtained in a straightforward way (see Fig. 4) and are listed in Table I.

Let us now discuss the results. First we observe that the exponents satisfy the scaling relation Eq. 1, confirming the validity of the scaling ansatz for this quantum phase transition. The exponents $\beta$, $\nu$ and $\eta$ are in excellent 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.

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 not only the mean field universality class suggested by Ref. [11], but also the Ising universality class (see Table I for a comparison).

This excellent agreement is a strong numerical support for the conjecture of Chubukov, Sachdev and Ye [2] that the Berry phase terms in the 2D QAFM are indeed dangerously irrelevant. To further confirm their predictions we have calculated the uniform susceptibility close to criticality down to $T = 0.02$, more than an order of magnitude lower than Ref. [7]. We have 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 excellent agreement with the above estimate. The linear slope is $\Omega_1(\infty)(J_0/hc)^2 = 0.238 \pm 0.003$. By extrapolating the spin wave velocity determined in the ordered phase by the Hasenfratz-Niedermayer fit to the critical point we get $hc/J = 1.04 \pm 0.02$ and thus $\Omega_1(\infty) = 0.26 \pm 0.01$, again in excellent agreement with Chubukov et al. [2] (see Tab. II).

To summarize, we have calculated the critical exponents of the quantum critical point in a planar antiferromagnet by a large scale quantum Monte Carlo study. Our exponents agree perfectly 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. The conjecture that all quantum phase transitions between a Néel ordered and a quantum disordered state in 2D Heisenberg antiferromagnets, whether they contain Berry phase terms or not, are in the same universality class as the quantum nonlinear sigma model is strongly supported.

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FIG. 1. Lattice structure of the 1/5-th depleted square lattice of CaV_{4}O_{9}. The dashed square indicates the eight spin unit cell used in our calculations.

\[
\frac{\xi}{L} = 0.936, 0.937, 0.938, 0.939, 0.94, 0.95
\]

FIG. 2. Plot of the ratio of correlation length divided by system size \(\xi/L\). 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 Eqns. (3) and (4).

\[
\beta = 0.345 \pm 0.021, 
\nu = 0.695 \pm 0.032
\]

FIG. 4. Staggered magnetization \(m_s\) and spin stiffness \(\rho_s\) calculated by a fit of the low temperature susceptibilities on finite lattices to the Hasenfratz-Niedermayer equations [16]. The straight lines are fits used to obtain the exponents \(\beta\) and \(\nu\).
TABLE I. Critical exponents $\beta$, $\nu$, $\eta$ and $z$. Listed are both the estimates 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              | $\nu$   | $\beta$  | $\eta$   | $z$           |
|--------------------|---------|----------|----------|---------------|
| 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       |         | 0.03 ± 0.01 | 1.08 ± 0.05 |
| 3D O(3)            | 0.7048 ± 0.0030 | 0.3639 ± 0.0035 | 0.034 ± 0.005 | —              |
| 3D Ising           | 0.6294 ± 0.0002 | 0.326 ± 0.004  | 0.0327 ± 0.003 | —              |
| mean field         | 1       | 1/2       | 0        | 1              |

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 the present study.

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