Asymptotic scaling of the square lattice quantum Heisenberg antiferromagnet

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We present thermodynamic measurements of various physical observables of the two dimensional S=1/2 isotropic quantum Heisenberg antiferromagnet on a square lattice, obtained by quantum Monte Carlo. In particular we have been able to measure the infinite volume limit of the uniform susceptibility up to the inverse temperature β = 40, the analysis of which reveals the correct asymptotic behavior in excellent agreement with the prediction of chiral perturbation theory. The issue of the existence of a crossover from quantum critical to renormalized classical regime is clarified.

75.40Mg, 75.10Jm, 75.40 Cx, 05.70Jk

The square lattice quantum Heisenberg antiferromagnet (QHA) is important in condensed matter physics since it describes the critical behavior of undoped insulating parent compounds of the high Tc superconductors. Some materials believed to be well described by these models are La$_2$CuO$_4$ \[\text{(2+1)D} O(3)\] and K$_2$NiF$_4$, also La$_2$NiO$_4$ \[\text{(2+1)D} O(3)\] and K$_2$NiF$_4$. Most existing theoretical treatments of the long wavelength, low energy behavior of the QHA are actually based on an effective field theory, the (2+1)D $O(3)$ non-linear σ model (NLσM). Although the mapping from the QHA to the NLσM may be justified on the general ground of universality, it is rigorous only for sufficiently large values of the magnitude of the quantum spin (S). There is also a subtle problem due to the existence of Berry phase terms, which are present in the effective field theory of the QHA, but not in the NLσM. This term is believed not to be relevant, but this is still a matter of debate.

The results of previous experimental and numerical studies on the S=1/2 QHA show a leading exponential temperature dependence of the correlation length, in agreement with the prediction of the theories (2+1)D $O(3)$ and numerical simulations (2+1)D $O(3)$. There nevertheless exist some systematic discrepancies between the observed values and theoretical predictions: the two-loop order formula of the correlation length deviates by more than 15% from both measurements and numerical simulations. The deviation becomes worse as the value of S increases, in contrast to naive expectations. Recent neutron scattering experiments on Sr$_2$CuO$_2$Cl$_2$, which is regarded as a more ideal realization of the S=1/2 QHA than the previously used compound La$_2$CuO$_4$, show systematic deviations from the theoretical prediction for the peak value of the static structure factor. The presence of a crossover from quantum critical to renormalized classical behavior predicted by the theories remains controversial with differing claims reported in the literature.

In this Letter we present results of a very large scale quantum Monte Carlo study on the S=1/2 square lattice QHA up to the linear size of the lattice $L=1000$. Our study resolves the above discrepancies, and clearly confirms the validity of the theory. Using the continuous time version of the loop algorithm that eliminates the systematic error due to finite Suzuki-Trotter number, we measure the thermodynamic values of various physical observables such as the uniform susceptibility, staggered susceptibility, second moment correlation length, peak value of the staggered structure factor $S_Q$ at $Q=(\pi,\pi)$ and internal energy. For each $T$ and $L$ we performed $10^6 \sim 10^7$ single loop updates after thermalization.

In order to monitor finite size effects in our measurements, we repeated the measurements at each temperature with varying lattice size and found that the measured values of the staggered susceptibility, $S_Q$, become size independent under the condition $L/\xi \gtrsim 7$, within the typical relative statistical errors of 0.3 percent or better. This condition is very restrictive for the measurements of the infinite volume limit values of various physical observables such as the uniform susceptibility $\chi_u$, staggered susceptibility $\chi_s$, and peak value of the staggered structure factor $S_Q$ at $Q=(\pi,\pi)$.

A selection of our data is shown in Table 1. The complete data will be presented in a forthcoming publication. In the following we discuss our measurements and fit them to theoretical predictions.

**Uniform susceptibility.** Chiral perturbation theory predicts (with convention $J = \hbar = g_B = k_B = 1$ hereafter)

$$\chi_u^{HN} = \frac{2}{3} \chi_\perp \left[ 1 + \frac{T}{2\pi \rho_s} + \left( \frac{T}{2\pi \rho_s} \right)^2 \right]$$

(1)

where $\chi_\perp = \rho_s/c^2$. It turns out that the fit of our data to

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Eq. (4) becomes stable only for data with $\beta \geq 4.5$, with $\chi^2/N_{DF} \simeq 0.6$. The estimated values of the parameters from the fit are

$$\rho_s = 0.179(2), \quad c = 1.652(1).$$

These values are in remarkably good agreement with those obtained from spin wave theory of the QHA [16].

Our estimate of $\chi_\perp$ is

$$\chi_\perp = 0.0656(1),$$

which is also consistent with the result of the spin wave theory [10].

Also predicted theoretically [8] is a crossover from quantum critical behavior to renormalized classical one, that is, from [8]

$$\chi_u = \frac{1}{c^2} [A_u T + B_u(\rho_s)]$$

to Eq. [8]. In Eq. [8] the constant $A_u$ is universal. The best estimate from QMC is $A_u = 0.26 \pm 0.01$ [8]. $B_u$ is only known to leading order in a $1/N$ expansion [8] as $B_u \approx 0.57\rho_s$. We observe (Fig. 1) that in a reasonably broad range $0.3 \lesssim T \lesssim 0.5$ $\chi_u$ is linear in $T$ with the expected slope $A_u$ and an offset $B_u \approx 0.47\rho_s$, reasonably close to the analytical estimate.

**Internal Energy:** We find that the energy $E$ becomes size independent under the condition $L/\xi \gtrsim 3$. Our measurements are over $0.25 \leq \beta \leq 5.5$, usually by varying $\beta$ by 0.25, on lattices of size up to $L=1000$. The theoretical prediction given in Ref. [8] is

$$E(T) = E_0 + E_3 T^3 + E_5 T^5, \quad E_3 = \frac{2\zeta(3)}{\pi c^2}. \tag{5}$$

Due to considerable uncertainties in three parameter fits, we here fix the value of $E_3$ with the value of $c$ given from the fit of $\chi_u$, i.e., $c = 1.652$ rather than treating $E_3$ as a fitting parameter. It turns out that only data for $\beta \gtrsim 4.25$ fit reasonably well to Eq. (3) with $\chi^2/N_{NF} \simeq 1.0$. We observe however that the fit is still slightly unstable in the sense that the values of the fitting parameters change mildly with the range of $T$ selected for the fit. The ground state energy we have extracted is

$$E_0 = -0.66953(4), \tag{6}$$

which may be compared with $E_0 = -0.6693 \sim -0.6694$ obtained from the ground state properties of QHA [17,18]. Due to the mild increasing tendency of $E_0$ with restricting the fit to lower temperatures, our estimate (Eq. (6)) may be regarded as a weak lower bound of the correct value.

**Correlation Length:** The prediction of $\xi$ from the two loop order of the chiral perturbation theory up to the first order of $T$ reads [8]

$$\xi_{HN} = \frac{e}{8} \frac{c}{2\pi\rho_s} \exp \left( \frac{2\pi\rho_s}{T} \right) \times \left[ 1 - \frac{T}{4\pi\rho_s} \right]. \tag{7}$$

We measured the infinite volume limit $\xi$ over the inverse temperature range $0.25 \leq \beta \leq 4.95$, corresponding to $0.289(2) \leq \xi \leq 120.5(4)$, and fitted our data to Eq.
\[ \rho_s = 0.185(1), \quad c = 1.442(3). \]  

(8)

Due to the systematic tendency this value of \( \rho_s (c) \) should be regarded as the upper (lower) bound of the correct asymptotic value. Although those extracted from our \( \chi_u \) data , Eq. (4), are indeed consistent with the the bounds, our \( \xi \) over \( 0.25 \leq \beta \leq 4.95 \) strongly deviate from the asymptotic expression (Fig. 2). However we wish to note that both our data and the experimental measurements can be fitted quite well by Eq. (4) with the correct \( \rho_s \) if one leaves the prefactor a free fitting parameter, as was done in Ref. 2.

The theory also predicts a crossover from the behavior in the quantum critical regime, given by \( \chi / \xi (T) = A_{QC} \pi / \xi + B_{QC} \xi / T \), to the asymptotic behavior Eq. (6). The expressions for \( A_{QC} \) and \( B_{QC} \) were obtained to one-loop order of the renormalization group calculation \( 14 \). A previous Monte Carlo study \( 11 \) claimed that all \( \xi \) fit a simple exponential form even for \( \beta \) as low as 0.25, contrary to our data. They thus concluded that there is no crossover. On the other hand a series expansion study \( 12 \) claimed to see a crossover \( 12 \). We indeed observe that \( 1 / \xi \) is linear in \( T \) over \( 1.273(6) \leq \xi \leq 3.25 \), but the measured values of \( A_{QC} \) and \( B_{QC} \) are not consistent with the theoretical predictions \( 14 \). Moreover, we observe such a linearity even in the 2D classical Heisenberg model where there should be no such crossover. Our data are not consistent with the one-loop order equations for the crossover regime \( 13 \) either. Thus our results seem incompatible with the scenario of a crossover in \( \xi \).

The peak value of the static structure factor: Theory \( 13 \) predicts for low \( T \)

\[ \frac{S_Q(T)}{\xi^2(T)} = A 2 \pi M^2 \left( \frac{T}{2 \pi \rho_s} \right)^2 \left( 1 - C \frac{T}{2 \pi \rho_s} \right), \]  

(9)

with a universal constant \( A \). \( M \approx 0.307 \) \( 13 \) is the ground state magnetization. However the experimental data suggested \( 2, 9 \) that \( S_Q(T)/\xi^2(T) \) is temperature independent over the temperature range accessible in the experiment.

We find that the data at \( \xi \geq 8.4 \) fit with an acceptable \( \chi^2/N_{DF} = 0.9 \) (see Fig. 3). The estimated value of \( C = -0.6(1) \) suggests that the effect of the correction term is less than one percent for \( T \leq 0.02 \), which may be regarded as the asymptotic regime for Eq. (4). For the universal prefactor we get the estimate \( A \approx 4.0 \). A series expansion study \( 12 \) got \( A_{1/2}^* \approx 3.2 \) for spin \( S = 1/2 \) and \( A_{\infty}^* \approx 6.6 \) for spin \( S = \infty \). Our result clearly shows, that as conjectured in Ref. 12, these values do not agree because the models are not yet in the low-\( T \) scaling regime. As the fits are unstable in the sense that \( A \) increases as we leave out data at higher \( T \) in the fit we view our estimate as a lower bound.

We wish to note that for \( \xi \geq 2.37(1) \) our data also fits to \( S_Q(T)/\xi^2(T) \sim T^N \) with \( N \approx 1.85(3) \) with an acceptable value of \( \chi^2/N_{DF} \approx 0.75 \).

Our data are definitely in agreement with the theory but not with the analysis from experiment 2. The comparison with experimental data will be discussed in more detail in a forthcoming publication 14.

The staggered susceptibility: In the classical high-\( T \) and in the low-\( T \) renormalized classical regime the staggered susceptibility is expected to be related to the staggered structure factor as \( 3 \)

\[ \frac{S_Q}{T \chi_{ST}} = 1. \]  

(10)

This prediction agrees with QMC measurements by Sandvik et al. \( 20 \). Our data, shown in Fig. 4 also confirm it, with even higher precision. In the quantum critical regime this ratio is expected to be also constant but with a value of \( 20 \)

\[ \frac{S_Q}{T \chi_{ST}} \approx 1.09. \]  

(11)

Instead of an expected plateau with this value the data however show a peak with a maximum around \( T \approx 0.8 \) \( 20 \). While the peak value is close to the predicted quantum critical regime the temperature is outside the range
where quantum critical behavior is observed in the uniform susceptibility. Thus we hesitate to ascribe this maximum to quantum critical behavior.

**Conclusion and discussion:** We believe that we have presented for the first time a set of thermodynamic data which displays the asymptotic behavior predicted by chiral perturbation theory. The values of the spin-stiffness constant and spin wave velocity agree well with those given by the spin wave theory of the QHA. This agreement is truly remarkable since the chiral perturbation theory is on the NLrM whereas the spin wave theory is on the QHA. Our results strongly confirm the validity of the map from the QHA to the NLrM in describing the long distance behavior of the former. Our estimates of $\rho_s$ and $c$ from the analysis of $\chi_u$ may be compared with previous estimates based on the size dependence formula near the ground state, i.e., $\rho_s = 0.185(2)$ and $c = 1.68(1)$ \cite{1}. They are extracted, however, by three parameter fits, which generally involve rather large uncertainties in estimates.

The fact that the asymptote of $\chi_u$ manifests itself only at such low temperatures may account for previous puzzles raised in studies of the correlation length. The deviation of $\xi$ from Eq. (7) is reduced to approximately 10 percent at $\beta \approx 4.9$ from the 20 percent deviation seen previously at $\beta = 2.5$. In fact this is similar to the 2D classical Heisenberg model as demonstrated by recent numerical studies \cite{21,22}. Our data of $S_Q$ and $\chi_u$ also indicate that one needs to probe data with much lower $T$ for the correction term to be safely ignored.

Another puzzle raised in experimental \cite{2,3} and numerical \cite{12} studies was: why is the agreement of the measurements worse for larger spins $S$? Equation (7) depends on the value of $S$ only implicitly through the $S$-dependence of $\rho_s$ and $c$. The reason for the larger discrepancies at larger $S$ is implicit in the assumptions in the theory: it is valid only for $\frac{\rho_s}{\pi T} << 1$ and $\frac{\rho_s}{\pi T} \ll \frac{\pi T}{\rho_s} \sim 1/S$. The latter condition restricts the validity of the theory to larger and larger correlation lengths as the spin $S$ is increased.

We also clarify the issue of the existence of the crossover. As suggested in Ref. \cite{6} the uniform susceptibility, where all logarithmic corrections in the theory cancel, shows a clear crossover from a quantum critical to the renormalized classical regime around $T \sim J/3$. In all other quantities however no good evidence for a crossover can be observed.

After completing our simulations, we became aware of a recent related preprint \cite{23} that addresses similar subjects. The authors claim to extract thermodynamic $\xi$ up to $\beta = 12$, with corresponding $\xi$ of order of $10^5$, based on recently developed finite size scaling extrapolation methods \cite{21a}. This finite size scaling method requires the existence of a universal scaling function that has no explicit $T$ dependence. The existence of this function can be explicitly checked numerically. However, contrary to the corresponding classical case \cite{21}, we observed, in a high-precision study, that in this quantum spin system the scaling function becomes approximately $T$ independent only when $T$ is very small. Detailed accounts of this issue will appear in a separate paper \cite{24}.

The simulations were performed on the 1024-node Hitachi SR2201 massively parallel computer of the computer center of the University of Tokyo and used about 250,000 hours of CPU time. M.T. was supported by the Japanese Society for the Promotion of Science.

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TABLE I. A selection of thermodynamic data for the 2D QHA in the range $0.25 \leq \beta \leq 4.95$. 

| $\beta$  | $0.25$ | $1.75$ | $2.25$ | $2.75$ | $3.25$ | $3.75$ | $4.25$ | $4.75$ | $4.95$ |
|----------|--------|--------|--------|--------|--------|--------|--------|--------|--------|
| $\xi$    | 0.289(2)| 2.37(1) | 4.46(1) | 8.38(1) | 15.7(1) | 29.0(1) | 52.8(2) | 95.7(3) | 120.5(4) |
| $\chi_{st}$| 0.0811(2)| 4.185(7) | 12.54(3) | 38.2(1) | 117.3(3) | 357.5(9) | 1082(3) | 3230(10) | 4980(17) |
| $\chi_u$ | 0.0487(1) | 0.0840(1) | 0.0735(1) | 0.0656(1) | 0.0604(1) | 0.0572(1) | 0.0550(1) | 0.0535(1) | 0.0531(1) |
| $\xi$    | -0.0986(1) | -0.5609(1) | -0.6162(1) | -0.6432(1) | -0.6559(1) | -0.6618(1) | -0.6648(1) | -0.6663(1) | -0.6676(1) |
| $S_Q$    | 0.329(1) | 2.63(1) | 5.96(1) | 14.40(2) | 36.91(5) | 95.7(2) | 254.8(5) | 682(2) | 1007(5) |

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