Quantum 2D Heisenberg antiferromagnet: bridging the gap between field-theoretical and semiclassical approaches

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The field-theoretical result for the low-\(T\) behaviour of the correlation length of the quantum Heisenberg antiferromagnet on the square lattice was recently improved by Hasenfratz [Eur. Phys. J. B 13, 11 (2000)], who corrected for cutoff effects. We show that starting from his expression, and exploiting our knowledge of the classical thermodynamics of the model, it is possible to take into account non-linear effects which are responsible for the main features of the correlation length at intermediate temperature. Moreover, we find that cutoff effects lead to the appearance of an effective exchange integral depending on the very same renormalization coefficients derived in the framework of the semiclassical pure-quantum self-consistent harmonic approximation: The gap between quantum field-theoretical and semiclassical results is here eventually bridged.

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In the last two decades, thermodynamic properties of the quantum Heisenberg antiferromagnet on the square-lattice (QHAF) have been determined by a number of substantially different methods. Theoretical predictions were compared with experimental data for real compounds [1], as well as with numerical simulations obtained by different methods [2, 3], and also with high-\(T\) series expansions [4]. Despite this effort, however, a comprehensive picture of the subject has not yet been formulated.

Much of the analysis and debate on the QHAF has focused on the temperature- and spin-dependence of the staggered correlation length \(\xi(T, S)\). Goal of this paper is to show that \(\xi(T, S)\) can be expressed as

\[
\xi(T, S) = \xi_{cl}\left(\frac{T}{J_{eff}(T, S)}\right), \tag{1}
\]

where the effective exchange integral \(J_{eff}(T, S)\) embodies quantum effects and is defined in terms of purely quantum spin-fluctuations, while \(\xi_{cl}(T/J_{cl})\) is the correlation length of the classical HAF. In particular, we find that Eq. (1), besides being the outcome of the semiclassical pure-quantum self-consistent harmonic approximation (PQSCHA) [5], remarkably holds also for the quantum field-theoretical prediction [6], as recently improved by Hasenfratz [7]. On the other hand, we show that the PQSCHA, when properly designed to such purpose, allows for a correct description of the low-\(T\) regime, via the appearance of the very same \(J_{eff}(T, S)\) implicitly entering Hasenfratz’s expression.

It is a definite suprise that a typical semiclassical expression such as Eq. (1), come out of a field-theoretical result, especially in the case of the QHAF, where semiclassical and field-theoretical approaches seemed destined to describe different regions of the \((T, S)\) plane, with no possible overlap.

The QHAF is defined by the spin Hamiltonian

\[
\hat{\mathcal{H}} = \frac{J}{2} \sum_{i \neq d} \hat{S}_i \cdot \hat{S}_{i+d}, \tag{2}
\]

where \(J > 0\), \(i = (i_1, i_2)\), \(d = (\pm 1, \pm 1)\), and lengths are in lattice units; the spin operators \(\hat{S}_i = (\hat{S}_i^x, \hat{S}_i^y, \hat{S}_i^z)\) satisfy \(|\hat{S}_i|^2 = S(S+1)\).

The correlation length \(\xi(T, S)\) is defined via the asymptotic behaviour, \(\lim_{|r| \rightarrow \infty} G(r) \propto e^{-|r|/\xi}\), of the staggered correlation function \(G(r) = (-1)^{r_1 + r_2} \langle \hat{S}_i^z \hat{S}_{i+r}^z \rangle\), with \(r = (r_1, r_2)\) any vector on the square lattice.

The classical counterpart of the QHAF corresponds to the limit \(S \rightarrow \infty\) with \(JS^2 \rightarrow J_{cl}\), that gives the classical Hamiltonian \(\mathcal{H} = (J_{cl}/2) \sum_{i \neq d} s_i \cdot s_{i+d}\), where \(s_i\) are classical unit vectors and \(J_{cl}\) is the only energy scale of the model.

Let us consider the right-hand side of Eq. (1): The 3-loop analytical expression for the classical correlation length, as from the field-theoretical approach [8], is

\[
\xi_{cl}(3l)\left(\frac{T}{J_{cl}}\right) = \frac{1-\pi/2}{8\sqrt{32}} \frac{T}{2\pi J_{cl}} \frac{2\pi J_{cl}}{\pi} \left[1 - \frac{0.574}{2} \right] + O(T^2). \tag{3}
\]

This expression is quantitatively correct up to \(T/J_{cl} \lesssim 0.4\). Above this temperature it smoothly connects to the exact Monte Carlo data for the classical model [8], so that the exact classical correlation length \(\xi_{cl}(T/J_{cl})\) gets available for all temperatures.

As for the left-hand side of Eq. (1), the most celebrated field-theoretical result is the 3-loop expression derived from the correlation length of the quantum nonlinear \(\sigma\)-model (QNL\(\sigma\)M) [9],

\[
\xi_B(T, S) = \frac{c}{8\pi^2} e^{\frac{2\pi J_{cl}}{T}} \left[1 - \frac{1}{2}\right] + O(\frac{T^2}{S^4}). \tag{4}
\]
The mapping to the QHAF consists of identifying $c$ and $\rho_s$ with the zero-$T$ renormalized spin velocity and spin stiffness of the system

$$ c = 2\sqrt{2}JSZ_c(S), \quad \rho_s = JS^2Z_\rho(S), \quad (5) $$

with $Z_c(S)$ and $Z_\rho(S)$ quantum renormalization coefficients; for $c$ and $\rho_s$ we will hereafter use the most accurate available values \cite{10}, as from their expansion up to $O(S^{-2})$ and $O(S^{-3})$, respectively.

One of the essential features of Eq. (4) is the temperature-independent pre-exponential factor $(c/\pi)(c/2\pi\rho_s)$, which contrasts with the $O(T)$ prefactor of the classical Eq. (3). The $O(1)$ prefactor gives a purely exponential asymptotic behaviour $\xi \sim e^{A/\xi}$, with $A \sim 2\pi JS^2$, which is also the outcome of other theoretical methods such as the Schwinger-boson approach \cite{11} and the modified spin-wave theory \cite{12}. Thus the behaviour $\xi \sim e^{A/\xi}$ has been generally regarded as a signature of the quantum character of the model. Early numerical studies suggested this signature is observed in the experimentally accessible temperature region of $S = 1/2$ antiferromagnets \cite{13}. In the last few years, however, this assumption has proved misleading in subtle ways, as severe difficulties arose when approaching the $S \geq 1$ case by the effective field-theory. Finally, in Ref. \cite{2} it was clearly shown that Eq. (4) holds only for temperatures low enough to ensure an extremely large correlation length, e.g., $\xi \gtrsim 10^5$ for $S = 1$, $\xi \gtrsim 10^{12}$ for $S = 3/2$, and generally cosmological correlation lengths for $S > 3/2$.

In Ref. \cite{2} Hasenfratz explained why cutoff effects, which are so devious for $S = 1/2$, significantly modify the correlation length for $S \geq 1$. By exploiting a direct mapping between the QHAF and the QNLrM, Hasenfratz obtained the cutoff-corrected field-theoretical result

$$ \xi_H(T, S) = \xi_{cl}(T, S) e^{-C(T, S)}, \quad (6) $$

where $C(T, S)$, defined in Eq. (14) of Ref. \cite{1}, is an integral of familiar spin-wave quantities over the first Brillouin zone. With this correction, which is the leading order in the spin-wave expansion for the cutoff correction, it is possible to obtain numerically accurate results down to $\xi \gtrsim 10^3$ for all $S$. Eq. (6) is therefore the best available prediction of the field-theoretical approach.

Our first step is to note that the function $C(T, S)$ may be written as

$$ C(T, S) \equiv \frac{\pi}{2} + \ln \frac{16JS\zeta_1(0, S)}{T} - 2\pi JS^2\zeta_1(0, S) \left[ \delta\zeta_1(T, S) + \delta\zeta_0(T, S) \right], \quad (7) $$

where $\delta\zeta_1(T, S) = \zeta_1(T, S) - \zeta_1(0, S) = O(T/S^2)$, and

$$ \zeta_1(T, S) = 1 + \frac{1}{2S} \frac{1}{2SN} \sum_k (1 - \gamma_k)^{1/2} L_k(T, S), \quad (8) $$

$$ \zeta_1(0, S) = 1 + \frac{1}{2S} \frac{1}{2SN} \sum_k (1 - \gamma_k)^{1/2} L_k(T, S), \quad (9) $$

$$ \zeta_1(0, S) = 1 + \frac{1}{2S} \frac{1}{2SN} \sum_k (1 - \gamma_k)^{1/2} L_k(T, S), \quad (10) $$

with sums over wavevectors $k = (k_1, k_2)$ in the first Brillouin zone, and $\gamma_k = (\cos k_1 + \cos k_2)/2$.

From the above formulas we find

$$ \xi_H(T, S) = A_1(T, S) \xi_{cl}(T, S) \left( \frac{T}{JS^2} \right) A_2(T, S) \xi_3(T, S), \quad (11) $$

with

$$ A_1(T, S) = \frac{2\pi}{\pi^2} e^{2\pi JS^2 \zeta_0(0, S)}, \quad A_2(T, S) = \frac{2\pi}{\pi^2} \zeta_1(0, S) \left[ \delta\zeta_1 + \delta\zeta_0 \right], \quad A_3(T, S) = \left[ 1 - \frac{T}{JS^2} \left( \frac{1}{2S} - 0.574 \right) + O\left( \frac{T^2}{S^2} \right) \right]; $$

notice that $A_1$ is an exact coefficient, while $A_2$ is given at the first order in $1/S$ as from Ref. \cite{2}, this is a signature of the different approaches used in determining $\xi_H$ and $C(T, S)$. As for $A_3$, it contains the 3-loop correction terms of the field-theoretical results.

In order to single out the relevant temperature scale in the exponential factor of Eq. (11), one can embody the $O(S^{-1})$ terms of the leading exponential in the argument of $\xi_{cl}(T, S)$: to this end we explicitly write $Z_\rho$ and $Z_c$ from their spin-wave theory expression \cite{10}

$$ Z_c = \zeta_1(0, S) + \Delta Z_c, \quad Z_\rho = \zeta_1(0, S)\zeta_0(0, S) + \Delta Z_\rho, \quad (12) $$

where $\Delta Z_c$ and $\Delta Z_\rho$ are $O(S^{-2})$, and find

$$ \xi_H(T, S) = \xi_{cl}(T, S) \left( \frac{T}{J_{eff}(H)}(T, S) \right) \alpha(T, S) \quad (13) $$

with

$$ J_{eff}(H)(T, S) = JS^2 \zeta_0(T, S) \zeta_1(T, S), \quad (14) $$

$$ \alpha(T, S) = \left[ 1 + \delta\zeta_1 + \delta\zeta_0 + O(S^{-2}) \right] \times \left[ 1 - \frac{T}{JS^2} \left( \frac{1}{2S} - 0.574 \right) + O\left( \frac{T^2}{S^2} \right) \right]. \quad (15) $$

At this level, the classical correlation length enters Eq. (13) by its 3-loop NLrM expression, Eq. (3). However, inspired by the PQLSCHA result of Ref. \cite{1} we are led to generalize Eq. (13) by replacing $\xi_{cl}(T, S)$ with the exact $\xi_{cl}$, which is numerically available at all temperatures. This is a fundamental step in order to get Eq. (13) to reproduce the experimental and quantum Monte Carlo (QMC) data in the intermediate temperature range, a goal that Eq. (13) does not accomplish yet.

In Fig. 4 we show the ratio $\xi_H/\xi_{cl}$ as a function of $T/JS^2$ for $S = 5/2$. The solid line is obtained by replacing $\xi_{cl}(T, S)$ in Eq. (13) with the exact $\xi_{cl}$. Compared with Hasenfratz’s expression (dash-dotted line), the agreement with
our QMC data greatly improves, just because the classical correlation length is accounted for exactly.

It is worthwhile mentioning that one could use the exact $\xi_{cl}$ already in Eq. (11) (dotted line in Fig. 1) - such curve shows that the pronounced minimum in the ratio $\xi/\xi_{cl}$, a feature that field-theoretical results do not reproduce, is due to substantially classical nonlinear effects which need a non-perturbative (or exact) treatment; this is confirmed by comparing the classical exact $\xi_{cl}$ (thin solid) and 3-loop $\xi_{cl(3)}$ (thin dash-dotted) lines, reported in Fig. 1 by fixing $J_{eff}$ to the classical limit ($L_0=0$) of $J_{eff(H)}$. The correct position of the minimum, on the other hand, is found by properly singling out the dominant temperature scale for the quantum correlation length, i.e., by determining the appropriate effective exchange integral. To this respect, by comparing Eq. (14) with Eqs. (5) and (12), one can see that $J_{eff(H)}(T,S)$ tends to $\rho_s$ for $T\rightarrow 0$ and can be actually interpreted as a temperature-dependent spin stiffness $\rho_s(T)$.

Finally, we drop the 3-loop correction terms, set the residual $\alpha(T,S)$ to unity, and eventually obtain Eq. (11), with the effective exchange integral Eq. (11). The corresponding curve is shown in Fig. 1 by the thin dashed line. The anomalous behaviour seen as $T\rightarrow 0$ has no physical meaning: in fact, when considering $\xi$ as in Eq. (11) with $J_{eff(H)}$, the ratio $\xi/\xi_{cl}$ contains a vanishing factor $\exp(-2\pi JS^2\Delta Z_\rho/T)$, due to the fact that $\rho_s$ in $\xi_{cl}$ is taken up to $O(S^{-3})$, while $J_{eff(H)}$ is only taken up to $O(S^{-2})$. To this respect, it is worthwhile noticing that Hasenfratz’s expression (11) is spurious as far as the order in $1/S$ is concerned, because $C(T,S)$ and $\xi_{cl}$ are accurate up to $O(S^{-1})$ and $O(S^{-3})$, respectively. This originates few other inconsistencies in the $1/S$ approximation, essentially contained in the $O(S^{-2})$ terms of Eq. (13), which result in slight discrepancies from the expected values. Nevertheless, the thin dashed line reproduces the behaviour drawn by QMC data in the whole temperature range and bridges the low- and intermediate-$T$ regime, a success never scored before.

Let us now comment on the above result. First of all, we notice that $J_{eff(H)}$ depends just on the pure-quantum part of the spin-fluctuations, i.e., the difference between the quantum and the classical spin-fluctuations (12) (the signature of this being the Langevin functions Eq. (13)). In particular, the renormalization factors $\zeta_0(T,S)$ and $\zeta_1(T,S)$ represent the effect of the pure-quantum fluctuations of each spin with respect to its local alignment axis and to its nearest-neighbors, respectively.

By considering Eq. (13) with the low-$T$ expansions

$$
\delta\zeta_0(T,S) \approx \frac{T}{2\pi JS^2\zeta_1(0,0)} \ln \frac{16JS\zeta_1(0,0)}{T} + O(T^3),
$$

$$
\delta\zeta_1(T,S) \approx \frac{T}{4JS^2\zeta_1(0,0)} + O(T^3),
$$

one sees that it is the pure-quantum on-site renormalization parameter $\zeta_0(T,S)$ that cancels the classical-like pre-exponential factor. This suggests that the asymptotic behaviour of Eq. (13) sets in when pure-quantum fluctuations of one spin relative to its nearest neighbors become negligible, and spins are mainly affected by on-site fluctuations of pure-quantum origin.

At this point, we recall that the pure-quantum renormalization coefficients $\zeta_0(T,S)$ and $\zeta_1(T,S)$ are characteristic of the PQSCHA, by which the correlation length of the QHAF in the form of Eq. (11) was first obtained (5) with

$$
J_{eff}(T,S) = JS^2\zeta_1^2(T,S) .
$$

The resemblance between Eqs. (11) and (16) is remarkable, given the fact that the PQSCHA is a completely different method from that used by Hasenfratz. However, the PQSCHA fails to describe the regime of very low-$T$, e.g., for $S=1/2$ it holds only for $T \geq 0.2 J$. In particular, the PQSCHA has been criticized because the expression Eq. (16) does not lead to the correct low-$T$ asymptotic behaviour of $\xi$. In fact, we here show that the PQSCHA may be properly designed to describe the low-$T$ regime, thus reproducing Eq. (13), though with $c$ and $\rho_s$ only given at the first order in $1/S$. This is an essential issue, as it means that the QHAF, even in the low-$T$ limit, is a system with separable classical and pure-quantum aspects.

One of the main steps in deriving the PQSCHA for a magnetic system is the construction of an effective classical spin Hamiltonian from that written in terms of canonical variables (14). For the sake of clarity, we use $(p,q)=(p_i,q_i)$ and $s=(s_i)$ to indicate the set of classical
canonical variables and unit vectors, respectively, needed to describe the classical system (see Ref. 3 for detailed definitions). For the partition function of the QHAF one finds \( Z = \int dp dq \exp(-\mathcal{H}(p, q)_{\text{eff}}/T) \)

\[
\mathcal{H}_{\text{eff}}(p, q) = \theta^4 \mathcal{H}(\frac{p}{\theta}, \frac{q}{\theta}) \rightarrow \theta^4 \mathcal{H}(s)
\]

and \( \theta^2 \equiv (1 + 1/2s)^{-1} \); the further scaling \( p \rightarrow \theta p \) and \( q \rightarrow \theta q \) reproduces the classical-like Heisenberg Hamiltonian \( \mathcal{H}(s) = \sum_i s_i s_{i+\ell} \), thus defining \( J_{\text{eff}} \) as in Eq. (10). When the correlation functions are considered, different scaling laws come into play, via the integral

\[
G(r) \propto \int dp \ dq \ g_{\text{eff}}(r; p, q) \ e^{-\mathcal{H}_{\text{eff}}(p, q)/T}
\]

where \( g_{\text{eff}} \) scales according to

\[
g_{\text{eff}}(r; p, q) = \theta^4_r \ g(r; s_{\theta r}) \rightarrow \theta^4_r \ g(r; s)
\]

with \( g(r; s) = N^{-1} \sum r s_i s_{i+r} \). \( \theta^2_r \) is a pure-quantum renormalization coefficient defined in Ref. 3. As both \( \mathcal{H}(p, q) \) and \( g(r; p, q) \) are biquadratic functions, the different scalings (with \( \theta \) or \( \theta_r \)) conflict. At intermediate \( T \), thermodynamics is governed by many different spin configurations, and the effective Hamiltonian appearing in the Boltzmann factor in Eq. (18) dominates (i.e., scaling with \( \theta \) is preferable \[5\]): this gives Eq. (16). At low-\( T \) the quartic terms in the effective Hamiltonian do not renormalize \( p \) and \( q \) to the bare frequencies originally used by Hasenfratz. In fact, the PQSCHA method \[3, 14\] uses even more refined temperature- and configuration-dependent renormalized frequencies; treating them within the so-called low-coupling approximation yields a more accurate finite-\( T \) expression, which is crucial for quantitative accuracy in evaluating thermodynamic quantities \[3\].

In this paper we have shown that, when cutoff effects are properly taken into account, the field theoretical expression for the correlation length of the QHAF analytically contains its classical counterpart, according to a simple equation that gives the former in terms of the latter with an effective exchange integral. Such equation surprisingly holds at all temperatures. Once the exact classical correlation length is available, the above result is used to make clear that the main features of the quantum correlation length at intermediate temperatures are due to essentially classical non-linear effects, which cannot be taken into account by perturbative approaches. Moreover, the effective exchange integral is seen to depend on the same pure-quantum renormalization coefficients defined by the PQSCHA, according to an expression which is very similar (equal) to that found by the latter approach in its standard (low-\( T \)) version.

The idea that an effective exchange integral may be uniquely defined for all thermodynamic quantities of the QHAF, as predicted by the PQSCHA, is suggestive and deserves, in our opinion, further investigation by the field-theoretical community.

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