Quantum versus classical behavior in the boundary susceptibility of the ferromagnetic Heisenberg chain

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We calculate the temperature dependence of the boundary susceptibility $\chi_B$ for the quantum ferromagnetic Heisenberg chain by a modified spin-wave theory (MSWT). We find that $\chi_B$ diverges at low temperatures $\sim -T^{-3}$ and therefore more rapidly and with opposite sign than the bulk susceptibility $\chi_{bulk} \sim T^{-2}$. Our result for $\chi_B$ is identical in leading order with the result for the classical system. In next leading orders, however, quantum corrections to the classical result exist which are important to obtain a good description over a wide temperature range. For the $S = 1/2$ case, we show that our full result from MSWT is in excellent agreement with numerical data obtained by the density-matrix renormalization group applied to transfer matrices. Finally, we discuss the quantum to classical crossover as well as consequences of our results for experiment in some detail.

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I. INTRODUCTION

Although the classical and the quantum version of the ferromagnetic Heisenberg model have the same ground state, it is not obvious in how far the low temperature properties of these systems are also similar. The Hamiltonian for the quantum ferromagnetic chain with open boundary conditions (OBC), spin $S$ and $N$ sites in a magnetic field $h$ along the $z$-direction is given by

$$H = -J \sum_{n=1}^{N-1} S_n S_{n+1} - g \sum_{n=1}^{N} h S_n^z$$

(1)

where $J > 0$ is the coupling constant and $g$ the g-factor. The classical version of this model can be obtained by introducing new unit vector operators $s_n = S_n/S$. These new operators commute in the limit $S \to \infty$, leading to the classical Hamiltonian

$$H = -J_c \sum_{n=1}^{N-1} s_n s_{n+1} - g_c \sum_{n=1}^{N} h_s n^z.$$  

(2)

To allow for a comparison between the quantum and the classical Hamiltonian for different spin values $S$ we have set $J_c = JS^2$ and $g_c = gS$.

The finite temperature properties of the classical model had been calculated several decades ago for OBCs as well as periodic boundary conditions (PBC). Whereas the first correction to the total free energy in the thermodynamic limit for PBC is $O(1/N)$, the free energy for OBC contains a term $O(1)$. This boundary or surface free energy then yields $O(1)$-contributions to all other thermodynamic quantities as for example the susceptibility. From Fisher’s results one finds that the classical bulk susceptibility behaves as

$$\chi_{bulk} = Ng_c^2 \left( \frac{2J}{3T^2} - \frac{1}{3T} \right)$$

(3)

whereas the classical boundary susceptibility ($O(1)$ contribution) is given by

$$\chi_B = -g_c^2 \left( \frac{2J_c^2}{3T^3} - \frac{4J_c}{3T^2} + \frac{1}{3T} \right).$$

(4)

$\chi_B$ therefore diverges more rapidly and with opposite sign than $\chi_{bulk}$.

A very different behavior for bulk and boundary susceptibility has also recently been observed for the quantum antiferromagnetic $S = 1/2$ XXZ-chain with anisotropy $0 \leq \Delta \leq 1$. For this system it is known that the bulk susceptibility is finite for $T \to 0$ with the $T = 0$ value of $\chi_{bulk}$ depending on the anisotropy $\Delta$. $\chi_B(T)$, on the other hand, is finite only for $0 \leq \Delta < 1/2$ whereas it diverges for $1/2 \leq \Delta \leq 1$ when $T \to 0$. By a combination of different techniques like bosonization, conformal field theory, Bethe ansatz as well as numerical results, a complete picture of the low-temperature properties of $\chi_B$ has been obtained. These results are not only of theoretical interest but might also be relevant for realizations of quasi one-dimensional antiferromagnets as for example SrCuO$_2$, in particular, when such compounds are doped with a moderate amount of non-magnetic impurities. In such a case the spin chain will be partitioned into finite chains with essentially free boundaries and knowledge of the boundary contributions will be essential to understand experiments on such systems.

For the quantum $S = 1/2$ ferromagnetic chain the standard bosonization approach and conformal field theory are not applicable because the dispersion relation is quadratic instead of linear. The model is, however, still...
integrable and thermodynamic properties can in principle be calculated either by the thermodynamic Bethe ansatz (TBA) or by the Bethe ansatz applied to quantum transfer matrices. The bulk susceptibility has indeed been obtained by an analysis of the TBA equations. In the first analysis of this kind by Schlottmann, it has been proposed that $\chi_{\mathrm{bulk}} \sim J/T^2 \ln(J/T)$. A later numerical analysis of the TBA\cite{6,9,10}, however, showed that $\chi_{\mathrm{bulk}} \sim J/6T^2$ at low temperatures as in the classical case but with corrections to this leading term which are different from Eq. (3). In addition it has been found that the leading term as well as the quantum corrections can be obtained by a modified spin-wave theory (MSWT)\cite{11}. It has been later shown that the classical and quantum ferromagnetic chains obey the same scaling laws at low temperatures\cite{12}. Furthermore, the critical theory controlling the low-energy behavior of both chains has been identified, which explains in more general terms why $\chi_{\mathrm{bulk}}$ and $\chi_{\mathrm{bulk}}$ are identical at low temperatures\cite{12,13}.

It is still unclear how the TBA has to be modified to allow also for the calculation of boundary contributions. Some of the difficulties one encounters are discussed in Refs.\cite{14, 15}. Within the QTM approach an explicit formula for the boundary free energy has been derived very recently\cite{16}. The explicit evaluation of this formula, however, is still a formidable task because it involves expectation values of an operator in the dominant eigenstate of the QTM which are notoriously difficult to calculate.

For these reasons we will follow here a different route and will use in section II Takahashi’s MSWT, which has been so successful for the bulk, to calculate the boundary susceptibility. In section III we then compare our result with numerical data obtained by the density-matrix renormalization group applied to transfer matrices (TMRG). In the last section we discuss the quantum to classical crossover observed and comment on the relevance of our results for experiment.

II. MODIFIED SPIN-WAVE THEORY

With the help of the Holstein-Primakoff transformation

$$S_n^+ = \sqrt{2S} \left(1 - a_n^\dagger a_n\right)/2S a_n , \quad S_n^- = S - a_n^\dagger a_n \quad (5)$$

the model\cite{11} can be represented exactly in terms of bosons $a_n$. Linear spin-wave theory is obtained if one replaces the second square root in Eq. (5) by 1. Corrections to this simple approximation can be calculated in principle in a systematic way by expanding the square root in powers of $1/S$. In any of these approximations it is important to notice that the bosons have to obey a hard-core constraint restricting the maximum number of bosons per site to $2S$. In higher dimension it is often acceptable to ignore this constraint completely. In one dimension, however, this constraint is crucial but hard to incorporate locally. Because the $SU(2)$ symmetry in a system with $h = 0$ can only be broken at $T = 0$ we might instead try to introduce a constraint which fixes the number of bosons to be $S$ on the average so that

$$\frac{1}{N} \sum_n \langle S_n^z \rangle = 0 \quad (6)$$

at any finite temperature. This approach has been used successfully by Takahashi\cite{6} to calculate the free energy and the susceptibility for a chain with PBC. We will use the same approach here for a system with OBC to obtain the boundary susceptibility.

Let us first rederive Takahashi’s result for PBC in a slightly different way. Expanding up to quartic order in the boson operators in Eq. (6) and using a one-loop approximation for the quartic terms, we obtain for the Hamiltonian\cite{11} at zero magnetic field

$$H = JS' \sum_k \epsilon(k) a_k^\dagger a_k + \nu \sum_k a_k^\dagger a_k$$

$$\epsilon(k) = 2(1 - \cos k) \quad (7)$$

and the average number of bosons $n_k$ is given by

$$n_k := \langle a_k^\dagger a_k \rangle = [\exp(JS'\epsilon(k)/T + \nu) - 1]^{-1} \quad (9)$$

At temperatures $T/J < 1$ the number of bosons in high momentum states is small. The bosons in low momentum states, on the other hand, will yield only a small contribution to the sum in Eq. (8) so that we will set $S' = S$ in the following. According to Eq. (4), the potential $\nu$ then has to be determined in such a way that

$$S = \frac{1}{N} \sum_k n_k \quad (10)$$

Differentiating the partition function for the Hamiltonian\cite{11} twice with respect to $h$ one finds that the susceptibility is given by

$$\chi = \frac{g^2}{2T} \sum_{n,m} \langle S_n^z S_m^z \rangle \quad (11)$$

However, the spin-wave expansion we are using here breaks the $SU(2)$ symmetry so that we will calculate the susceptibility instead by

$$\chi = \frac{g^2}{3T} \left\{ \sum_{n=1}^N \sum_{m \neq n} \langle S_n S_m \rangle + NS(S + 1) \right\} \quad (11)$$

In this way the consequences of $SU(2)$ symmetry breaking are less severe due to the averaging over all three directions. Using the constraint\cite{10} one finds\cite{6}

$$\langle S_n S_m \rangle = \left( \frac{1}{N} \sum_k \cos[k(r_n - r_m)]n_k \right)^2 \quad (12)$$
The momenta for a chain of length \( N \) with PBC are given by \( k = 2\pi l/N \) where \( l = 0,1,\ldots,N-1 \). For \( T/J \ll 1 \) the most important contributions to the sum in (12) come from \( k \approx 0,2\pi \) and we can evaluate these contributions by using a saddle point integration

\[
\langle S_n S_m \rangle \approx \left( \frac{1}{2\pi} \int_0^{2\pi} \frac{\cos[k(r_n - r_m)]}{e^{JS\xi(k)+v} - 1} dk \right)^2
\]

\[
\approx \left( \frac{T}{JS\pi} \int_0^\infty \frac{\cos[k(r_n - r_m)]}{k^2 + Tv/JS} dk \right)^2
\]

\[
= \frac{t}{4\nu} \exp(-2\sqrt{\nu}|r_n - r_m|).
\]

In the last line we have introduced the abbreviation \( t = T/JS \). To understand why the saddle point approximation for the integrand in (13) is indeed sufficient here we make the following observation: (13) can be evaluated alternatively by closing the integration contour in the upper or lower half of the complex \( k \)-plane, depending on the sign of \( r_n - r_m \). The residues closest to the real axis then yield (14). Next-leading residues give contributions \( O(\sqrt{T} \exp[-\sqrt{T}]) \). These would result in terms \( O(1/\sqrt{T}) \) in the susceptibility, which are neglected in the ongoing.

From the constraint (11) one can easily determine the potential \( \nu \) as a series in \( \sqrt{\nu} \). The result is

\[
\nu = \sqrt{\nu} + q \left( \frac{\nu}{2S} \right)^2 + q^2 \left( \frac{\sqrt{\nu}}{2S} \right)^3 + O(t^2),
\]

where \( q = (1/2)/\sqrt{\pi} \). When we rewrite the correlation function (13) in terms of the normalized spin operators \( s_n \) and the coupling constant \( J_n \), as given in the introduction and use only the leading term from (13) we find

\[
\langle s_n s_m \rangle = \exp(-|r_n - r_m|T/J_c)
\]

for all values of \( S \). In particular, the correlation length at \( T/J \ll 1 \) is always given by \( \xi = J_c/T \). Furthermore, Eq. (16) also agrees with the result for the classical model.\(^\text{1}\) Note, however, that this is no longer the case if one takes the next-leading terms in (16) into account.

To calculate the susceptibility we have to evaluate the sum in Eq. (11). For PBC each distance \( |r_n - r_m| = 1, \ldots, N/2 \) appears 2\( N \) times. The susceptibility in the thermodynamic limit can therefore be obtained by

\[
\chi_{\text{PBC}} = \lim_{N \to \infty} \frac{g^2}{3T} \left\{ \frac{N/t}{2\nu} \sum_{r=1}^{N/2} e^{-2\sqrt{\nu}r} + NS(S+1) \right\}
\]

\[
= \frac{Ng^2}{12JS} \left( t^{-1/2} \nu^{-3/2} - \nu^{-1} \right)
\]

\[
+ 4S(S+1)t^{-1} + O(e^{-N}).
\]

The first term agrees exactly with the result obtained by Takahashi,\(^\text{6}\) however, we find here in addition the second and third term, which are absent in Takahashi’s result. Note, that these terms exactly cancel each other for \( S \to \infty \). The differences between our and Takahashi’s result can be explained as follows: Whereas in Ref. 6 the sum in Eq. (11) is carried out \textit{without} approximating the correlation function (12) we have taken here only the long-distance asymptotics of \( \langle S_n S_m \rangle \) into account as obtained by the saddle point approximation in (13). Interestingly, the terms in the susceptibility up to \( O(1/T) \) remain unaffected, i.e., these terms are not influenced by the behavior of the correlation function at short-distances. In fact, we might trust our spin-wave approximation only in the long-wavelength limit where the spin-wave interaction is small. In our one-loop approximation this becomes clear when considering Eqs. (7,8). When all momenta involved are small, the sum in Eq. (8) is also small and \( S' \approx S \). In this limit the Hamiltonian (7) becomes equivalent to the one for ideal non-interacting spin waves.

For these reasons we cannot expect that the MSWT gives reasonable results if we try to calculate local quantities for OBC near the boundary. We observed that neither a local constraint \( \langle S_n^2 \rangle = 0 \) nor the correlation \( \langle S_n S_m \rangle \) can be calculated without inconsistencies. For example, if we calculate the correlation function for OBC explicitly we find a constant term which vanishes only if we set \( \nu = t/4\nu^2 \) exactly. However, the condition (10) still requires corrections to \( \nu \) as given in (16).

Far enough away from the boundaries, on the other hand, the correlation function will still behave as in Eq. (13). When we perform the sum in (11) using again this long-distance asymptotics for \( \langle S_n S_m \rangle \) but in a way appropriate for OBC we will already obtain a \( O(1) \) correction to the susceptibility \textit{without} taken the modifications to the correlation function near the boundary into account. We conjecture that for low temperatures, this term yields \( \chi_B \). The physical picture behind this procedure is as follows: We can combine two open chains each of length \( M - 1 \) to one periodic chain of length \( N = 2M \), where the two additional sites do not couple with their neighbors. We then carry out the sum in Eq. (11) only over one half of the periodic chain, thereby discarding correlations between this subsystem and the rest. Doing so we ignore local differences between PBC and OBC.

What makes us confident that this is indeed sufficient to obtain the leading terms in a low-temperature expansion for the boundary susceptibility \( \chi_B \) is that the leading term \( -1/T^3 \) is universal in the sense that it does not depend on \( S \). Especially, it is the leading term of \( \chi_B \) for both \( S = 1/2 \) and \( S = \infty \).\(^\text{12,13}\) The classical result for the correlation function (10) has been first obtained by Fisher\(^\text{4}\) for an open chain. I.e., in the classical limit the exponential decay of the correlation function does depend only on \( r_n - r_m \) and not on \( r_n, r_m \) alone, although translational invariance is broken!

We therefore conjecture that the leading terms in a low-temperature expansion of the susceptibility for a
quantum chain with OBC are given by

\[
\chi_{\text{OBC}} = \frac{g^2}{3T} \left\{ \frac{t}{2v} \sum_{n,m=1}^{N} e^{-2|r_n-r_m|\sqrt{vT}} + N S(S+1) \right\} \\
= \frac{Ng^2}{12JS} \left( t^{-1/2} v^{-3/2} - v^{-1} \right) \\
+ 4S(S+1)t^{-1} - \frac{1}{2N} t^{-1} v^{-2} + \mathcal{O}(e^{-N}) \tag{18}
\]

In particular, the boundary susceptibility is given by

\[
\chi_B = -\frac{g^2}{24JS} t^{-1} v^{-2} \\
= -\frac{g^2}{3Jt^3} \left( 1 - q^2 \frac{2\sqrt{t}}{S} + q^2 \frac{3t}{2S^2} + \ldots \right). \tag{19}
\]

Note that the leading term is identical to the leading term in the classical result \([1]\) when \(J, g\) are replaced by \(J_c, g_c\). This confirms our expectations. To test if the procedure proposed here gives indeed the right corrections to the classical result we will check formula (19) against numerical data for the \(S = 1/2\) quantum model in the following section.

### III. NUMERICAL RESULTS

In a system with OBC the one-point correlation function \(\langle S^z(r) \rangle\) is no longer a constant because translational invariance is broken. We define

\[
C(r) = \langle S^z(r) \rangle_{\text{OBC}} - m \tag{20}
\]

where \(m\) is the magnetization per site in the system with PBC and \(r\) is the distance from the boundary. The local boundary susceptibility is then given by \(\chi_B(r) = \partial C(r)/\partial h|_{h=0}\) and the total boundary susceptibility \(\chi_B\) can be obtained by

\[
\chi_B = \sum_{r=1}^{\infty} \chi_B(r) = \chi_{\text{OBC}} - \chi_{\text{PBC}}. \tag{21}
\]

This means that we can calculate \(\chi_B\) by considering only a local quantity which is particularly useful in numerical calculations where it is difficult to obtain the \(O(1)\) contribution directly. Particularly suited for this purpose is the density-matrix renormalization group applied to transfer matrices (TMRG) because the thermodynamic limit is performed exactly. The idea of the TMRG is to express the partition function \(Z\) of a one-dimensional quantum model by that of an equivalent two-dimensional classical model which can be derived by the Trotter-Suzuki formula.\([15,16]\) For the classical model a suitable transfer matrix \(T\) can be defined which allows for the calculation of all thermodynamic quantities in the thermodynamic limit by considering solely the largest eigenvalue of this transfer matrix. Details of the algorithm can be found in Refs.\([17,18,19,20]\) The method has been extended to impurity problems in Ref.\([21]\) In particular, the local magnetization at a distance \(r\) from the boundary of a system with \(N\) sites can be obtained by

\[
\langle S^z(r) \rangle = \frac{\sum_n \langle \Psi^0_R | T(S^z)T^{r-1} \tilde{T} T^{N-r}\Psi^0_L \rangle}{\sum_n \langle \Psi^0_R | T^{N-1}\tilde{T}\Psi^0_L \rangle} \tag{22}
\]

where \(|\Psi^0_R\rangle\) (\(|\Psi^0_L\rangle\) are the right (left) eigenstates of the transfer matrix \(T\), \(\tilde{T}\) is a modified transfer matrix containing the broken bond and \(T(S^z)\) is the transfer matrix with the operator \(S^z\) included. Because the spectrum of \(T\) has a gap between the leading eigenvalue \(\Lambda_0\) and the next-leading eigenvalues, Eq. (22) reduces in the thermodynamic limit to

\[
\lim_{N \to \infty} \langle S^z(r) \rangle = \frac{\langle \Psi^0_R | T(S^z)T^{r-1}\tilde{T}\Psi^0_L \rangle}{\Lambda_0 \langle \Psi^0_L | T \Psi^0_R \rangle}. \tag{23}
\]

Therefore only the leading eigenvalue and the corresponding eigenvectors have to be known to calculate the local magnetization in the thermodynamic limit. Far away from the boundary \(\langle S^z(r) \rangle\) becomes a constant, the bulk magnetization

\[
m = \lim_{r \to \infty} \lim_{N \to \infty} \langle S^z(r) \rangle \\
= \lim_{r \to \infty} \frac{\sum_n \langle \Psi^0_L | T(S^z)T^{r-1}\Psi^0_R \rangle \langle \Psi^0_R | T \Psi^0_L \rangle}{\Lambda_0} \tag{24}
\]

To obtain numerically the susceptibility profile \(\chi_B(r)\) we calculate \(C(r)\) for small fields \(h \sim 10^{-4}, 10^{-5}\) by using Eqs. (23,24) and then taking the numerical derivative.

Here we want to study the quantum model \([11]\) with \(S = 1/2, J = 1\) and \(g = 2\). First, we want to test our numerical results by calculating the bulk susceptibility and comparing with Eq. (17) which agrees with the TBA.\([22]\) The result is shown in Fig. 4 and the agreement at low temperatures is excellent. Note also, that although the leading terms in the low-temperature expansion for the classical and the quantum model are identical, extremely low temperatures are necessary to see the classical scaling for the \(S = 1/2\) quantum model.

The boundary susceptibility is shown in Fig. 2 in comparison to the classical result as well as to formula (19) conjectured for the quantum case. The excellent agreement confirms our conjecture for the \(S = 1/2\) case. As \([19]\) also agrees with the classical result in the limit \(S \to \infty\) we expect that our result is valid for all \(S\).

Finally, we show in Fig. 3 susceptibility profiles \(\chi_B(r)\) for different temperatures. As the total boundary susceptibility is given by Eq. (21) which, on the other hand, should be equal to \([19]\) we can even determine an analytic formula for \(\chi_B(r)\) and find

\[
\chi_B(r) = -\frac{g^2}{24JS} 2^2 \sqrt{\pi} - \frac{1}{2N} t^{-1} v^{-2} e^{-2r\sqrt{vT}}. \tag{25}
\]
FIG. 1: $\chi_{\text{bulk}}$ as a function of temperature. The circles denote the numerical data obtained by TMRG, the dashed line is the classical result from Eq. (3) and the solid line Takahashi’s result (17) obtained by MSWT.

FIG. 2: Boundary susceptibility $\chi_B$ as a function of temperature. The circles denote the numerical data obtained by TMRG, the dashed line is the classical result from Eq. (4) and the solid line our result (19) from MSWT.

FIG. 3: Susceptibility profile $\chi_B(r)$ at a distance $r$ from the boundary for different temperatures $T = 0.013, \cdots, 0.8$. The dots represent the numerical, the dashed lines the theoretical result according to Eq. (25).

IV. CONCLUSIONS

We want to emphasize that the boundary susceptibility is not a finite size quantity. It is defined as the difference in susceptibilities between a periodic chain and a chain with OBC in the thermodynamic limit. In fact, when we calculated $\chi_{\text{PBC}}$ and $\chi_{\text{OBC}}$ in section II we have ignored terms $\sim \exp(-2N\sqrt{tv})$. For a finite chain with OBC this is a valid approximation if $T/J > 1/4N$ and our results can be directly applied if this condition is fulfilled. At temperatures $T/J \sim 1/N$, where finite size corrections are sufficiently small to be ignored, we find a $\sim 25\%$ reduction of the total susceptibility in the open compared to the periodic system. This effect should therefore be relevant in susceptibility measurements on systems with non-magnetic impurities when the temperature $T/J$ becomes comparable to the concentration of impurities (inverse average chain length).

In this context we want to mention that the low-$T$ behavior of $\chi_{\text{PBC}}$ following from Eqs. (15,17) has been observed experimentally. Furthermore, controlled doping of quasi-one dimensional ferromagnets with both magnetic and non-magnetic defects is possible. Most interestingly, susceptibility measurements of diluted two-dimensional ferromagnets have revealed a one-dimensional behavior at the percolation threshold and an unexplained lowering of the susceptibility under the percolation threshold at low temperatures. It would be certainly interesting to try to understand these experiments in more detail in the light of the results presented here.

Finally, we want to address the question at which temperature scale the crossover from quantum to classical behavior occurs. Clearly, the system behaves classically at length scales much smaller than the correlation length $\xi = 1/2\sqrt{tv} \approx J_c/T$ where all spins are practi-
ally aligned. The length scale for fluctuations is set by the spin-wave wavelength $\lambda \sim \sqrt{J_c/T S}$. So we expect classical behavior when $\lambda \ll \xi$ which is true for all $S$ at sufficiently low temperatures. As expected, $\lambda$ becomes smaller with increasing $S$ whereas the correlation length $\xi$ does not change. Therefore the crossover temperature will increase with the spin quantum number $S$.

In summary, we have used a modified spin-wave theory - where a chemical potential guarantees zero magnetization at zero magnetic field for any finite temperature - to calculate the boundary susceptibility $\chi_B$ for the open spin-$S$ quantum ferromagnetic chain. We found that $\chi_B$ can be expanded in powers of $\sqrt{T}$ and that the leading term is given by $\chi_B \sim -1/T^3$ in agreement with the classical result. The quantum corrections to this classical result are, however, important to obtain a good description over a wide temperature range. We have verified our formula for the $S = 1/2$ case by comparing with numerical data obtained by the density-matrix renormalization group applied to transfer matrices and have found excellent agreement. We have been even able to derive an analytic formula for the local boundary susceptibility $\chi_B(r)$ which we also checked numerically. Most important, we have shown that $\chi_B$ at low temperatures is “universal”, in the sense that it is completely determined by the long-distance asymptotics of the two-point correlation function $\langle S_n S_m \rangle$.

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