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 χ_B for the quantum ferromagnetic Heisenberg chain by a modified spin-wave theory (MSWT). We find that χ_B diverges at low temperatures $\sim -T^{-3}$ and therefore more rapidly and with opposite sign than the bulk susceptibility $\chi_{\text{bulk}} \sim T^{-2}$. Our result for χ_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 (OBCs), spin S and N sites in a magnetic field h along the z direction is given by

$$H = -J\sum_{n=1}^{N-1} \boldsymbol{S}_n \boldsymbol{S}_{n+1} - g\sum_{n=1}^{N} hS_n^z, \tag{1}$$

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 $\boldsymbol{s}_n=\boldsymbol{S}_n/S$.[1] These new operators commute in the limit $S\to\infty$, leading to the classical Hamiltonian

$$H = -J_c\sum_{n=1}^{N-1} \boldsymbol{s}_n \boldsymbol{s}_{n+1} - g_c\sum_{n=1}^{N} hs_n^z. \tag{2}$$

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 (2) were calculated several decades ago for OBCs,[1] as well as periodic boundary conditions (PBCs).[2] Whereas the first correction to the free energy per lattice site f_{PBC} for PBCs is $\mathcal{O}(1/N^2)$, the free energy per lattice site f_{OBC} for OBCs contains a term $\mathcal{O}(1/N)$,

$$f_{\text{OBC}} = f_{\text{bulk}} + \frac{1}{N}F_B. \tag{3}$$

Here we will study the coefficient of the $\mathcal{O}(1/N)$ contribution F_B for $N\to\infty$, i.e., the boundary contribution to the free energy for an infinitely long chain. This boundary or surface free energy F_B then yields $\mathcal{O}(1/N)$ contributions to all other thermodynamic quantities such as, for example, the susceptibility. From Fisher's results[1] one finds that the classical bulk susceptibility behaves as

$$\chi_{\text{bulk}}^c = \left.\frac{\partial^2 f_{\text{bulk}}}{\partial^2 h}\right|_{h=0} = g_c^2\left(\frac{2J_c}{3T^2} - \frac{1}{3T}\right) \tag{4}$$

whereas the classical boundary susceptibility [$\mathcal{O}(1/N)$ contribution] is given by

$$\chi_B^c = \left.\frac{\partial^2 F_B}{\partial^2 h}\right|_{h=0} = -g_c^2\left(\frac{2J_c^2}{3T^3} - \frac{4J_c}{3T^2} + \frac{1}{3T}\right). \tag{5}$$

χ_B^c therefore diverges more rapidly and with opposite sign than χ_{bulk}^c.

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 $0\leqslant\Delta\leqslant 1$.[3–5] For this system it is known that the bulk susceptibility is finite for $T\to 0$ with the $T=0$ value of χ_{bulk} depending on the anisotropy Δ. $\chi_B(T)$, on the other hand, is finite only for $0\leqslant\Delta<1/2$ whereas it diverges for $1/2\leqslant\Delta\leqslant 1$ 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 χ_B has been obtained.[3–5,27] These results are not only of theoretical interest but might also be relevant for realizations of quasi-one-dimensional antiferromagnets such as, for example, Sr_2CuO_3, in particular, when such com-

pounds are doped with a moderate amount of nonmagnetic 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[6] (TBA) or by the Bethe ansatz applied to quantum transfer matrices (QTMs).[7] The bulk susceptibility has indeed been obtained by an analysis of the TBA equations. In the first analysis of this kind by Schlottmann[8] it has been proposed that $\chi_{\text{bulk}} \sim J/T^2 \ln(J/T)$. A later numerical analysis of the TBA,[6,9,10] however, showed that $\chi_{\text{bulk}} \sim J/6T^2$ at low temperatures as in the classical case but with corrections to this leading term which are different from Eq. (4). 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).[6,11] It has later been shown that the classical and quantum ferromagnetic chains obey the same scaling laws at low temperatures.[12] Furthermore, the critical theory controlling the low-energy behavior of both chains has been identified, which explains in more general terms why χ^c_{bulk} and χ_{bulk} are identical at low temperatures.[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. 5 and 14. Within the QTM approach an explicit formula for the boundary free energy has been derived very recently.[14] 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 Sec. II Takahashi's MSWT, which has been so successful for the bulk, to calculate the boundary susceptibility. In Sec. 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

$$S_n^+ = \sqrt{2S}\sqrt{1 - a_n^\dagger a_n/2S}\; a_n, \quad S_n^z = S - a_n^\dagger a_n \tag{6}$$

the model (1) 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. (6) 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 potential V in the Hamiltonian, which fixes the number of bosons to be S on the average so that

$$\frac{1}{N}\sum_n \langle S_n^z \rangle = 0 \tag{7}$$

at any finite temperature. This approach has been used successfully by Takahashi[6] to calculate the free energy and the susceptibility for a chain with PBCs. We will use the same approach here for a system with OBCs to obtain the boundary susceptibility.

Let us first rederive Takahashi's result for PBCs 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 (1) at zero magnetic field

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

$$\epsilon(k) = 2(1 - \cos k), \tag{8}$$

where

$$S' = S - \frac{1}{2N}\sum_k \epsilon(k) n_k. \tag{9}$$

The average number of bosons n_k is given by

$$n_k := \langle a_k^\dagger a_k \rangle = \{\exp[JS'\epsilon(k)/T + v] - 1\}^{-1}, \tag{10}$$

where $v = V/T$. At temperatures $T/J \ll 1$ 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. (9) so that we will set $S' = S$ in the following. According to Eq. (7), the potential v then has to be determined in such a way that

$$S = \frac{1}{N}\sum_k n_k. \tag{11}$$

Differentiating the partition function for the Hamiltonian (1) twice with respect to h one finds that the susceptibility is given by $\chi = g^2/T \sum_{n,m} \langle S_n^z S_m^z \rangle$. However, the spin-wave expansion we are using here breaks the SU(2) symmetry so that we will calculate the susceptibility instead by

$$\chi = \frac{g^2}{3T}\left\{\frac{1}{N}\sum_{n=1}^{N}\sum_{m\neq n}\langle \boldsymbol{S}_n \boldsymbol{S}_m \rangle + S(S+1)\right\}. \tag{12}$$

In this way the consequences of SU(2) symmetry breaking are less severe due to the averaging over all three directions. Using the constraint (11) one finds[6]

$$\langle \boldsymbol{S}_n \boldsymbol{S}_m \rangle = \left(\frac{1}{N}\sum_k \cos[k(r_n - r_m)] n_k\right)^2. \tag{13}$$

The momenta for a chain of length N with PBCs are given by $k = 2\pi l/N$ where $l = 0, 1, \ldots, N-1$. For $T/J \ll 1$ the most im-

portant contributions to the sum in Eq. (13) come from $k \approx 0, 2\pi$ and we can evaluate these contributions by using a saddle-point integration

$$\langle \boldsymbol{S}_n \boldsymbol{S}_m \rangle \approx \left(\frac{1}{2\pi} \int_0^{2\pi} \frac{\cos[k(r_n - r_m)]}{e^{\beta JS\epsilon(k)+v} - 1} dk \right)^2 \tag{14}$$

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

$$= \frac{t}{4v} \exp(-2\sqrt{tv}|r_n - r_m|). \tag{15}$$

In the last line we have introduced the abbreviation $t = T/JS$. To understand why the saddle-point approximation for the integrand in Eq. (14) is indeed sufficient here we make the following observation: Eq. (14) 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 Eq. (15). Next-leading residues give contributions $\mathcal{O}(\sqrt{T} \times \exp[-\sqrt{T}])$. These would result in terms $\mathcal{O}(1/\sqrt{T})$ in the susceptibility, which are neglected in the ongoing.

From the constraint (11) one can easily determine the potential v as a series in $\sqrt{t}$. The result is[6]

$$\sqrt{v} = \frac{\sqrt{t}}{2S} + q\left(\frac{\sqrt{t}}{2S}\right)^2 + q^2\left(\frac{\sqrt{t}}{2S}\right)^3 + \mathcal{O}(t^2), \tag{16}$$

where $q = \zeta(1/2)/\sqrt{\pi}$. When we rewrite the correlation function (15) in terms of the normalized spin operators $\boldsymbol{s}_n$ and the coupling constant J_c as given in the introduction and use only the leading term from Eq. (16) we find

$$\langle \boldsymbol{s}_n \boldsymbol{s}_m \rangle = \exp(-|r_n - r_m|T/J_c) \tag{17}$$

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. (17) also agrees with the result for the classical model.[1] Note, however, that this is no longer the case if one takes the next-leading terms in Eq. (16) into account.

To calculate the susceptibility we have to evaluate the sum in Eq. (12). For PBCs each distance $|r_n - r_m| = 1, \ldots, N/2$ appears $2N$ times. The susceptibility in the thermodynamic limit can therefore be obtained by

$$\chi_{\mathrm{PBC}} = \lim_{N\to\infty} \frac{g^2}{3T} \left\{ \frac{t}{2v} \sum_{r=1}^{N/2} e^{-2r\sqrt{tv}} + S(S+1) \right\}$$

$$= \frac{g^2}{12JS}[t^{-1/2}v^{-3/2} - v^{-1} + 4S(S+1)t^{-1} + \mathcal{O}(e^{-N})]. \tag{18}$$

The first term agrees exactly with the result obtained by Takahashi,[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 result and Takahashi's result can be explained as follows: Whereas in Ref. 6 the sum in Eq. (12) is carried out *without* approximating the correlation function (13) we have taken here only the long-distance asymptotics of $\langle \boldsymbol{S}_n \boldsymbol{S}_m \rangle$ into account as obtained by the saddle-point approximation in Eq. (15). Interestingly, the terms in the susceptibility up to $\mathcal{O}(1/T)$ 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. (8) and (9). When all momenta involved are small, the sum in Eq. (9) is also small and $S' \approx S$. In this limit the Hamiltonian (8) becomes equivalent to the one for ideal noninteracting spin waves.

For these reasons we cannot expect that the MSWT gives reasonable results if we try to calculate local quantities for OBCs near the boundary. We observed that neither a local constraint $\langle S_n^z \rangle = 0$ nor the correlation function $\langle \boldsymbol{S}_n \boldsymbol{S}_m \rangle$ can be calculated without inconsistencies. For example, if we calculate the correlation function for OBCs explicitly we find a constant term which vanishes only if we set $v = t/4S^2$ exactly. However, the condition (11) still requires corrections to v as given in Eq. (16).

Far enough away from the boundaries, on the other hand, the correlation function will still behave as in Eq. (15). When we perform the sum in Eq. (12) using again this long-distance asymptotics for $\langle \boldsymbol{S}_n \boldsymbol{S}_m \rangle$ but in a way appropriate for OBCs we will already obtain a $\mathcal{O}(1)$ correction to the susceptibility *without* taking the modifications to the correlation function near the boundary into account. We conjecture that for low temperatures, this term yields χ_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. (12) only over one half of the periodic chain, thereby discarding correlations between this subsystem and the rest. Doing so we ignore local differences between PBCs and OBCs.

What makes us confident that this is indeed sufficient to obtain the leading terms in a low-temperature expansion for the boundary susceptibility χ_B is that the leading term $\sim -1/T^3$ is universal in the sense that it does not depend on S. Especially, it is the leading term of χ_B for both $S = 1/2$ and $S = \infty$.[12,13] The classical result for the correlation function (17) has been first obtained by Fisher[1] for an *open chain*. That is, 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 OBCs are given by

$$\chi_{\mathrm{OBC}} = \frac{g^2}{3T} \left\{ \frac{t}{4vN} \sum_{\substack{n,m=1 \\ n \neq m}}^{N} e^{-2|r_n - r_m|\sqrt{tv}} + S(S+1) \right\}$$

$$= \frac{g^2}{12JS} \left(t^{-1/2}v^{-3/2} - v^{-1} + 4S(S+1)t^{-1} - \frac{1}{2N} t^{-1}v^{-2} + \mathcal{O}(e^{-N}) \right). \tag{19}$$

In particular, the boundary susceptibility is given by

$$\chi_B = -\frac{g^2}{24JS}t^{-1}v^{-2} = -g^2\frac{2S^3}{3Jt^3}\left(1 - q\frac{2\sqrt{t}}{S} + q^2\frac{3t}{2S^2} + \cdots\right). \tag{20}$$

Note that the leading term is identical to the leading term in the classical result (5) 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 (20) against numerical data for the $S=1/2$ quantum model in the following section.

III. NUMERICAL RESULTS

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

$$C(r) = \langle S^z(r)\rangle_{\mathrm{OBC}} - m, \tag{21}$$

where m is the magnetization per site in the system with PBCs 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 χ_B can be obtained by

$$\chi_B = \sum_{r=1}^{\infty} \chi_B(r) = N(\chi_{\mathrm{OBC}} - \chi_{\mathrm{PBC}}). \tag{22}$$

This means that we can calculate χ_B by considering only a local quantity which is particularly useful in numerical calculations where it is difficult to obtain the $\mathcal{O}(1)$ 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 $\mathcal{T}$ 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. 17–20. 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

$$\langle S^z(r)\rangle = \frac{\sum_n \langle \Psi_L^n|\mathcal{T}(S^z)\mathcal{T}^{r-1}\widetilde{\mathcal{T}}\mathcal{T}^{N-r-1}|\Psi_R^n\rangle}{\sum_n \langle \Psi_L^n|\mathcal{T}^{N-1}\widetilde{\mathcal{T}}|\Psi_R^n\rangle}, \tag{23}$$

where $|\Psi_R^n\rangle$ ($\langle\Psi_L^n|$) are the right (left) eigenstates of the transfer matrix $\mathcal{T}$, $\widetilde{\mathcal{T}}$ is a modified transfer matrix containing the broken bond, and $\mathcal{T}(S^z)$ is the transfer matrix with the operator S^z included. Because the spectrum of $\mathcal{T}$ has a gap between the leading eigenvalue Λ_0 and the next-leading eigenvalues, Eq. (23) reduces in the thermodynamic limit to

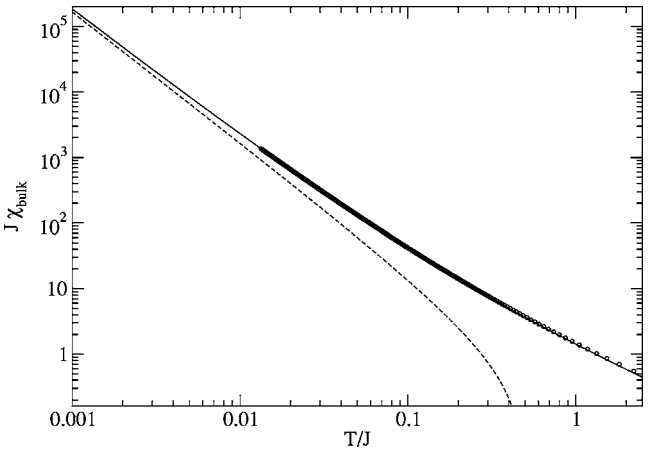

FIG. 1. χ_{bulk} as a function of temperature. The circles denote the numerical data obtained by TMRG, the dashed line is the classical result from Eq. (4), and the solid line Takahashi's result (18) obtained by MSWT.

$$\lim_{N\to\infty}\langle S^z(r)\rangle = \frac{\langle \Psi_L^0|\mathcal{T}(S^z)\mathcal{T}^{r-1}\widetilde{\mathcal{T}}|\Psi_R^0\rangle}{\Lambda_0^r\langle \Psi_L^0|\widetilde{\mathcal{T}}|\Psi_R^0\rangle}. \tag{24}$$

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

$$\begin{aligned} m &= \lim_{r\to\infty}\lim_{N\to\infty}\langle S^z(r)\rangle \\ &= \lim_{r\to\infty}\frac{\sum_n \langle \Psi_L^0|\mathcal{T}(S^z)\mathcal{T}^{r-1}|\Psi_R^n\rangle\langle\Psi_L^n|\widetilde{\mathcal{T}}|\Psi_R^0\rangle}{\Lambda_0^r\langle \Psi_L^0|\widetilde{\mathcal{T}}|\Psi_R^0\rangle} \\ &= \frac{\langle \Psi_L^0|\mathcal{T}(S^z)|\Psi_R^0\rangle}{\Lambda_0}. \end{aligned} \tag{25}$$

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. (24) and (25) and then taking the numerical derivative.

Here we want to study the quantum model (1) 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. (18), which agrees with the TBA.[6] The result is shown in Fig. 1 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 (20) conjectured for the quantum case. The excellent agreement confirms our conjecture for the $S=1/2$ case. As Eq. (20) 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

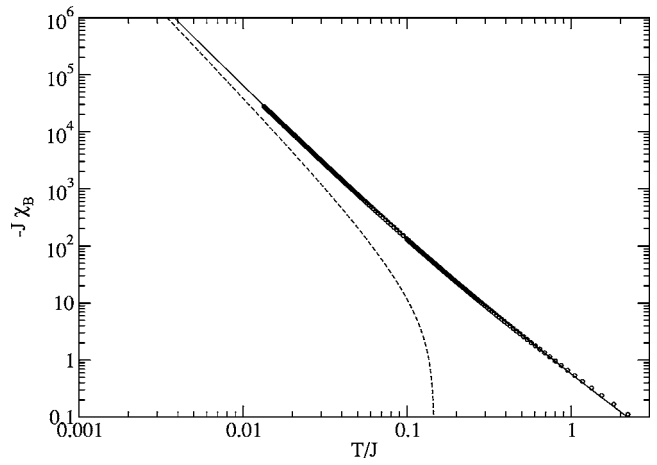

FIG. 2. Boundary susceptibility χ_B as a function of temperature. The circles denote the numerical data obtained by TMRG, the dashed line is the classical result from Eq. (5), and the solid line is our result (20) from MSWT.

given by Eq. (22) which, on the other hand, should be equal to Eq. (20) we can even determine an analytic formula for $\chi_B(r)$ and find

$$\chi_B(r) = -g^2 \frac{e^{2\sqrt{tv}} - 1}{24JS} t^{-1} v^{-2} e^{-2r\sqrt{tv}}. \tag{26}$$

This formula is in excellent agreement with our numerical data (see dashed lines in Fig. 3). The deviations at large distances r where $\chi_B(r)$ is small are due to numerical errors. For the fields $h \sim 10^{-5}$ used here, $\chi_B(r) \sim 10^{-2}$ corresponds to a local magnetization $C(r) \sim 10^{-7}$ which becomes comparable with the accuracy of the calculation. Note also that according to Eq. (26) the one-point correlation function $\langle S^z(r) \rangle$ will decay for small magnetic fields with exactly the same correlation length as the bulk two-point correlation function $\langle S^z(r) S^z(0) \rangle$. This connection between one- and two-point correlation functions has also been found for the antiferromagnetic XXZ chain.[5]

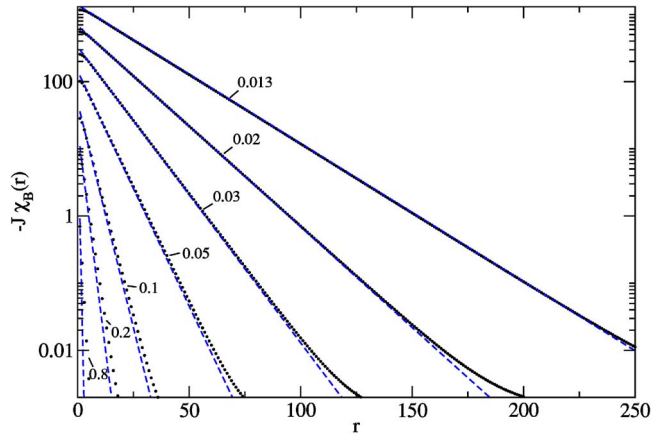

FIG. 3. (Color online) Susceptibility profile $\chi_B(r)$ at a distance r from the boundary for different temperatures $T=0.013, \ldots, 0.8$. The dots represent the numerical, the dashed lines the theoretical result according to Eq. (26).

IV. CONCLUSIONS

We want to emphasize that the boundary susceptibility calculated here is not a finite-size quantity. It is defined as N times the difference in susceptibilities between a periodic chain and a chain with OBCs in the *thermodynamic limit* $N \to \infty$. In fact, when we calculated χ_{PBC} and χ_{OBC} in Sec. II we ignored terms $\sim \exp(-2N\sqrt{tv})$. For a finite chain with OBCs 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 nonmagnetic 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 χ_{PBC} following from Eqs. (16) and (18) has been observed experimentally.[22,23] Furthermore, controlled doping of quasi-one-dimensional ferromagnets with both magnetic[24] and nonmagnetic[25] defects is possible. Most interestingly, susceptibility measurements of diluted two-dimensional ferromagnets have revealed a one-dimensional behavior at the percolation threshold,[26] and an unexplained lowering of the susceptibility under the percolation threshold at low temperatures. It would certainly be interesting to try to understand these experiments in more detail in the light of the results presented here. In addition, we like to point out that our numerical data show that at $T/J \sim 0.02$ the local susceptibility at the site closest to the boundary will be reduced by more than 40% and that a sizeable reduction (more than 10%) will extend over a distance of about 25 lattice sites from the boundary (impurity). We therefore expect that it should be possible to test our predictions for the local susceptibility directly by nuclear magnetic resonance Knight shift experiments.

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 practically aligned. The length scale for fluctuations is set by the spin-wave wavelength $\lambda \sim \sqrt{J_c/TS}$. So we expect classical behavior when $\lambda \ll \xi$, which is true for all S at sufficiently low temperatures. As expected, λ becomes smaller with increasing S whereas the correlation length ξ 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 χ_B for the open spin-S quantum ferromagnetic chain. We found that χ_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 even been 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 χ_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 $\langle \boldsymbol{S}_n \boldsymbol{S}_m \rangle$.

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