Spin correlations near the edge as probe of dimer order in square-lattice Heisenberg models

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Recent numerical and analytical work has shown that for the square-lattice Heisenberg model the boundary can induce dimer correlations near the edge which are absent in spin-wave theories and nonlinear sigma model approaches. Here, we calculate the nearest-neighbor spin correlations parallel and perpendicular to the boundary in a semi-infinite system for two different square-lattice Heisenberg models: (i) a frustrated J_1-J_2 model with nearest- and second-neighbor couplings and (ii) a spatially anisotropic Heisenberg model, with nearest-neighbor couplings J perpendicular to the boundary and J' parallel to the boundary. We find that in the latter model, as J'/J is reduced from unity, the dimer correlations near the edge become longer ranged. In contrast, in the frustrated model, with increasing J_2, dimer correlations are strengthened near the boundary but they decrease rapidly with distance. These results imply that deep inside the Néel phase of the J_1-J_2 Heisenberg model, dimer correlations remain short ranged. Hence, if there is a direct transition between the two, it is either first order or there is a very narrow critical region.

I. INTRODUCTION

Square-lattice antiferromagnets have been studied extensively in recent years.[1–9] Yet, new surprises continue to arise. In particular, recent quantum Monte Carlo studies by Höglund and Sandvik[10] showed that the existence of a free edge induces pronounced dimerized correlations in the system. In a follow up work, it was shown by Metlitski and Sachdev[11] that the presence of a boundary induces dimer correlations perpendicular to the boundary. Since the correlations decay with distance from the boundary, their gradient induces alternation in the spin correlations parallel to the boundary, leading to specific pattern of nearest-neighbor spin correlations observed by Höglund and Sandvik in their simulations. These effects are absent in spin-wave theories and in nonlinear sigma model approaches.

Over the past few years, there has been considerable interest in the possibility of direct continuous phase transitions between Néel and valence bond crystal (VBC) phases.[12–21] Such phase transitions have been called deconfined quantum criticality and are marked by the liberation of spin-half degrees of freedom as well as the existence of massless spin-singlet photon field. Strong numerical evidence for such a scenario has been provided in Sandvik's J-Q model,[22–24] where the Heisenberg model is supplemented by a four-spin interaction around a plaquette. An alternative possibility of a weakly first-order transition has also been raised.[25,26]

A more realistic model of two-dimensional square-lattice quantum antiferromagnets is the spin-half J_1-J_2 model, where there is nearest-neighbor interaction J_1 and second-neighbor interaction J_2. Increasing J_2 increases spin frustration and is known to lead to a magnetically disordered state at intermediate J_2/J_1 values.[5,7] There is substantial and growing body of numerical evidence that the magnetically disordered phase has VBC order.[2,3,7,12] The question of whether the transition between the Néel and dimer orders is continuous or first order remains a subject of debate.[27,28]

In general, it is difficult to probe the weak dimer correlations inside the Néel phase, which would require studying the connected part of the four-spin correlation functions. The existence of dimerization near the edges means that it is much easier to study the dimer correlations in the presence of an edge. Here, we would like to use the edge-induced dimer correlations as a probe of growth of dimer correlations inside the Néel phase and thus address the possibility of a diverging dimer-correlation length in the Néel phase. We study two models: a spatially anisotropic model with interactions J and J' along the two axes. We choose the boundary to be parallel to the direction of the weaker coupling J'. It is well known that the one-dimensional (1D) Heisenberg model has power-law decaying valence bond correlations. Thus, as one approaches the limit of small J', one expects to see the edge-induced correlations to have a long length scale. This model acts as a test case for our method. We also study the J_1-J_2 Heisenberg model. It is for this model that one would like to see how the range of dimer correlations grows near the boundary as spin frustration given by the parameter J_2/J_1 increases and one approaches the phase transition, where the Néel order is lost.

II. SERIES EXPANSION

The antiferromagnetic Heisenberg models defined by two coupling constants J_1 and J_2 (or by J and J') are shown in Fig. 1. We consider a semi-infinite (SI) system, with a boundary parallel to the X axis also shown in Fig. 1. Since we are considering a system inside a collinear Néel-ordered phase, we develop an Ising series expansion,[29] where all Heisenberg couplings are written as

$$\mathbf{S}_i \cdot \mathbf{S}_j = S_i^z S_j^z + \lambda (S_i^x S_j^x + S_i^y S_j^y). \qquad (1)$$

The parameter λ acts as an expansion parameter. We develop series expansions for on-site local magnetization $\langle S_i^z \rangle$ as well as for nearest-neighbor spin correlations $\langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle$, parallel and perpendicular to the boundary. In the semi-infinite system, these quantities depend on the distance R from the boundary. In the series-expansion method, the boundary can be accommodated by accounting for the graphs that terminate at the
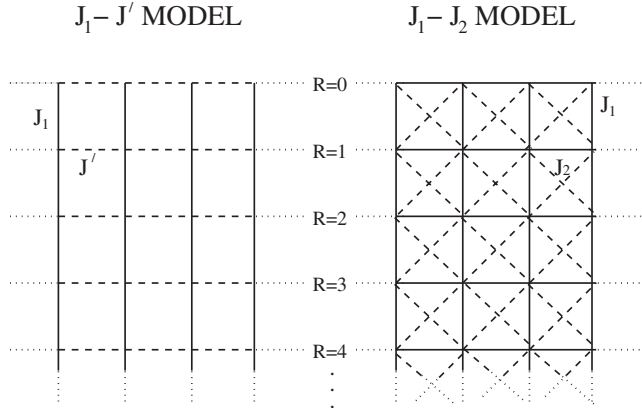
FIG. 1. (Left) J_1-J' model on the semi-infinite square lattice. The interaction $J_1=1$ is perpendicular to the edge, the interaction J' is parallel to the edge, and it is allowed to vary in the range $0 < J' \leq 1$. (Right) J_1-J_2 model on the semi-infinite square lattice. $J_1=1$ and $0 \leq J_2 < 0.3$. The parameter R defines the distance of a particular lattice plane from the edge.

boundary. Apart from this, the formalism of linked cluster expansions remains unchanged.

III. RESULTS: CORRELATIONS AND EXCITATIONS NEAR THE EDGE

First we present the results for the square-lattice Heisenberg model. The nearest-neighbor correlations parallel and perpendicular to the boundary are shown in Fig. 2. These are obtained by d-log Padé approximant analysis of the series. They agree well with the results of Sandvik and Höglund.[10] The important thing to note is that they both decrease rapidly with distance and by $R=5$ they differ from the bulk value by less than 0.1%.

The on-site magnetization also changes near the boundary. The results for magnetization are more sensitive to extrapolation methods than spin-spin correlations because one expects a square-root singularity for this quantity. This
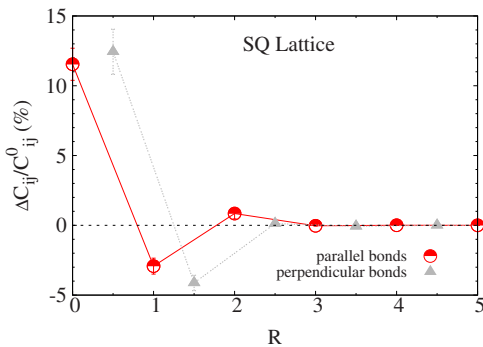

FIG. 2. (Color online) Correlation function of the spin-$\frac{1}{2}$ Heisenberg model on the SI square lattice for bonds parallel and perpendicular to the edge as a function of distance R. Notice that bonds perpendicular to the edge have their centers at half-integer values of R. The y axis is $\Delta C_{ij}/C_{ij}^0 = -\frac{\langle \vec{S}_i \cdot \vec{S}_j \rangle_{SI} - \langle \vec{S}_i \cdot \vec{S}_j \rangle_\infty}{\langle \vec{S}_i \cdot \vec{S}_j \rangle_\infty}$, where the ∞ index refers to the bulk value.
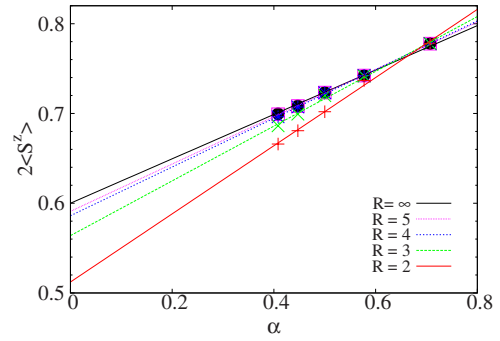

FIG. 3. (Color online) Partial sums of series-expansion coefficients for the on-site sublattice magnetization of the semi-infinite square-lattice model. The fit for different values of the parameter R is shown. See text for details.

means that contributions of higher-order terms only decay as $1/\sqrt{N}$. We have followed the method used in Ref. 30 for the bulk system. We obtain partial sums S_N of series coefficients and then fit them vs $\alpha = \frac{1}{\sqrt{1+N}}$ to estimate S_N as $N \to \infty$. These are shown in Fig. 3 for values of $R \geq 2$. We deduce the uncertainty in the magnetization by the uncertainty in the linear fits.

Results obtained this way are plotted in Fig. 4 where they are compared to the nonlinear σ model and spin-wave results.[11] The on-site sublattice magnetization is diminished at the edge and its reduction is comparable to what is obtained in spin-wave theory. Away from the edge, the sublattice magnetization should approach its bulk value. In the nonlinear σ model and spin-wave theory, the change in magnetization follows a $1/R$ behavior. On general grounds, one expects the nonlinear σ model results, when expressed in terms of renormalized parameters, to be exact[11] for large R. The reduction is less in our calculation up to the largest distance studied; that is, $R=5$. Part of the reason may be that the asymptotic behavior may set in at significantly large R due to the dimer correlations at the boundary. However, it is also likely that the uncertainty in our calculations is much larger than shown. Our estimate of the bulk magnetization is 0.302. If we replace it by the more accurate results from higher-order series expansions[9] or quantum Monte Carlo simulations,[22] which is 0.307, it would shift our calculated
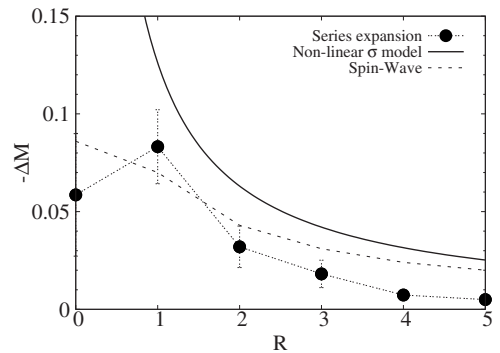

FIG. 4. On-site sublattice magnetization for the spin-$\frac{1}{2}$ Heisenberg model on the semi-infinite square lattice. The nonlinear sigma model and spin-wave results from Ref. 11 are also shown. The y axis is $\Delta M = (M_{SI} - M_\infty)$.
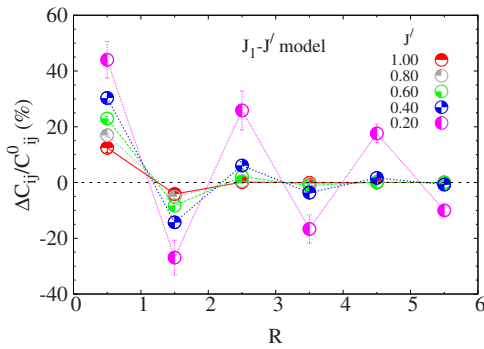
FIG. 5. (Color online) Correlation function of the spin-$\frac{1}{2}$ J_1-J' model on the semi-infinite square lattice for bonds perpendicular to the edge as a function of distance R for selected values of J'. The quantity $\Delta C_{ij}/C_{ij}^0$ shown on the y axis is defined in the caption of Fig. 2.

FIG. 7. Excitation spectrum of the Heisenberg model on the semi-infinite square lattice for $0 \leq k_x \leq \pi$, where k_x is the momentum parallel to the edge. The bound states found by spin-wave theory and series-expansion calculations are shown. The thin solid line represents the upper limit of the continuum of states.

curves up by 0.005 and bring them closer to the spin-wave results. This discrepancy in the bulk estimates implies that the uncertainties are much bigger than estimated by the fits and they are particularly magnified at larger R because we are taking the difference of two quantities which are close in magnitude.

In Fig. 5, we show the nearest-neighbor spin correlations perpendicular to the boundary for the J-J' model. This is the direction of the stronger coupling. In the 1D limit, one expects the free end to induce dimer correlations in the system that decay as a power law away from the boundary. Indeed, we find that as the system becomes more and more anisotropic, the dimer correlations become more and more long ranged.

In Fig. 6, we show the nearest-neighbor spin correlations for the J_1-J_2 model. Correlations both parallel and perpendicular to the boundary are shown. In this case, we find that while a frustrating second-neighbor interaction enhances the dimerization near the boundary, it does not appear to increase the range over which dimer correlations extend. The convergence of our analysis becomes poor as we get close to the bulk transition away from the Néel order, which has been estimated to be in the range $J_2/J_1 \approx 0.35-0.4$.[5,7,27]

These results show that in the J_1-J_2 square-lattice Heisenberg model, one does not have appreciable range valence bond correlation in the bulk even with significant frustration.
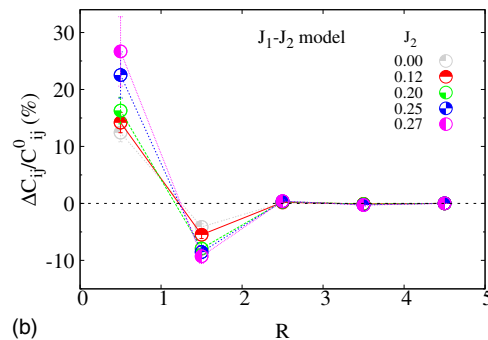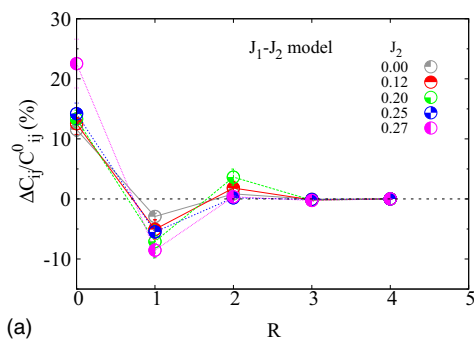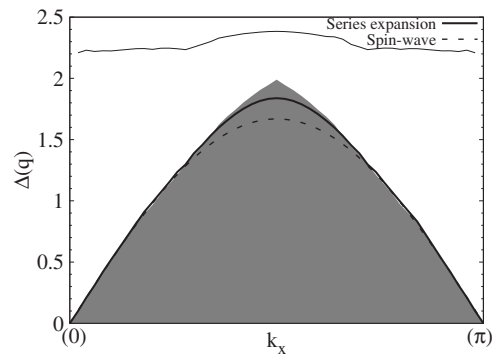
They suggest that a direct transition between Néel and dimer phases is likely of first order. Our study cannot rule out the possibility that the dimer correlations build up very quickly close to the transition. This would imply a very narrow critical region in this model.

We have also calculated the spin-wave spectrum for the magnon states that are bound to the surface for the nearest-neighbor square-lattice Heisenberg model. The momentum parallel to the surface is a good quantum number. In the series-expansion calculations, the spin-flip states right at the boundary have different excitation energies from those which are away from the boundary. Thus, these states get separated from the bulk states starting in zeroth order. Upon extrapolation to the Heisenberg model, we find the dispersion of these surface magnons as shown in the Fig. 7. Also shown are results from the spin-wave calculations of Metlitski and Sachdev.[11] The latter has been renormalized to have the same spin-wave velocity as the bulk. Our results are in agreement with the latter that for a large part of the Brillouin zone, the surface states are hugging the continuum. Only very near $k = \pi/2$, they clearly separate from the continuum. In this region, the binding energy in our calculation is smaller than in the spin-wave theory.

FIG. 6. (Color online) Correlation function of the spin-$\frac{1}{2}$ J_1-J_2 model on the semi-infinite square lattice for bonds parallel (a) and perpendicular (b) to the edge as a function of distance R for selected values of J_2. The quantity $\Delta C_{ij}/C_{ij}^0$ shown on the y axis is defined in the caption of Fig. 2.

IV. CONCLUSIONS

In this paper, we have studied the spin correlations and excitations near the boundary of two-dimensional Heisenberg antiferromagnets. Two different square-lattice models are considered: one where the exchange coupling parallel to the boundary is smaller than the one perpendicular to the boundary. In this model, we find that the boundary-induced dimerization becomes more and more long ranged as the anisotropy is increased. The second model is the J_1-J_2 Heisenberg model, with nearest- and second-neighbor exchange interactions. In this case, we find that as frustration is increased in the model, the boundary-induced dimerization increases close to the boundary but its range does not change significantly. This suggests that in the J_1-J_2 model, the Néel phase does not develop long-range dimer correlations. Hence, either the transition from Néel to dimer order is first order in this model or there is a very narrow critical region.

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