Critical entanglement of XXZ Heisenberg chains with defects

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We study the entanglement properties of anisotropic open spin one-half Heisenberg chains with a modified central bond. The entanglement entropy between the two half-chains is calculated with the density-matrix renormalization method (DMRG). We find a logarithmic behaviour with an effective central charge c' varying with the length of the system. It flows to one in the ferromagnetic region and to zero in the antiferromagnetic region of the model. In the XX case it has a non-universal limit and we recover previous results.

The consideration of entanglement properties has brought a new element into the study of many-particle quantum states. Entanglement is related to a division of the system into two parts and can be quantified via the reduced density matrix ρ and the entropy $S = -\mathrm{tr}(\rho \ln \rho)$ connected with it. This quantity is particularly interesting for the ground state of critical one-dimensional systems. For example, if one cuts an open chain into two halves of length L, conformal invariance predicts the universal form [1, 2]

$$S = \frac{c}{6} \ln L + k \tag{1}$$

where c is the central charge in the conformal classification. An analogous formula with $c/6$ replaced by $c/3$ holds for a segment of length L in an infinite chain. The logarithmic divergence is a particular signature of the criticality and can be related to analogous universal contributions to the free energy of critical two-dimensional systems with conical shape [2, 3, 4]. It has been verified numerically for a number of quantum chains [5, 6] and derived analytically for free fermions hopping on a chain [7]. For this system it can also be proven by putting proper bounds on S [8, 9].

Since the entanglement entropy measures the mutual coupling of the two parts of a system in the wave function, a defect at their boundary should have a strong influence. In one dimension, defects show particularly interesting features in Luttinger liquids, i.e. in strongly correlated fermionic systems. Their effective strength then depends on the sign of the interaction [10, 11] and goes to zero for attraction while it diverges for repulsion, as the system size increases. This has been checked in various further studies, see e.g. [12, 13, 14, 15, 16, 17]. One then wonders how the entanglement behaves in such a case and how the logarithmic law (1) is affected. This question was first raised by Levine [4] who used bosonization and found results to lowest order in the impurity strength which are consistent with the general picture. The simpler case of a free-fermion hopping model, corresponding to the XX spin chain, was treated numerically in Ref. [18]. In this case, the logarithmic behaviour was found to persist, but with a prefactor c_{eff} which depends continuously on the defect strength.

In the present paper we present a numerical study of this problem for the case of a planar XXZ spin chain, which has $c = 1$ and is the lattice version of a Luttinger model. We treat open chains with one modified bond in the middle and use density-matrix renormalization (DMRG) [19, 20]. This method is ideally suited for such a study since the calculation of ρ and its spectrum is an intrinsic part of the algorithm. We find that the effective central charge, which will be called c', tends asymptotically to one for $\Delta < 0$ (ferromagnetic region, resp. attraction) and to zero for $\Delta > 0$ (antiferromagnetic region, resp. repulsion). How fast this happens depends, however, on the defect strength, and for weak perturbations

and interactions the asymptotic region is still far away, although we treated chains up to 800 sites. We also compared to Levine's formulae but could not obtain a quantitative agreement, although we verify his general picture. In the following we first present the model and the method of calculation. Then we show some density-matrix spectra and their typical features. After that we present the calculations of S and the results for the quantity c' for a number of defect strengths J_{imp} and anisotropic parameters Δ. Finally we compare with Ref.[4] and draw our conclusions.

I. MODEL AND METHOD

We studied the XXZ model for an open chain of $2L-1$ sites, which is divided into a left part with L sites and a right part with $L-1$ sites. Both are connected by a bond of strength J_{imp} while for the rest of the chain we take $J=1$. The Hamiltonian then has the form

$$H = \sum_{i=1}^{L-1} h_i + J_{imp}\, h_L + \sum_{i=L+1}^{2L-2} h_i \tag{2}$$

where

$$h_i = \frac{1}{2}\left(S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+\right) + \Delta S_i^z S_{i+1}^z \tag{3}$$

and the anisotropy Δ lies between -1 and $+1$. Written in terms of spinless fermions, the S^zS^z-term corresponds to a nearest-neighbour interaction which is repulsive (attractive) for $\Delta > 0$ ($\Delta < 0$). The system was studied in its ground state which in the present case corresponds to total spin $S^z = \pm 1/2$, and we took $S^z = +1/2$. In the fermionic formulation, the filling is $L/(2L-1)$ and thus slightly above $1/2$. We chose the odd total length in order to avoid relatively large oscillations between even and odd L-values which are present in even-length chains. These are connected with the different dimerization patterns in the spin correlation functions which are induced by the open ends. Although this is an interesting topic, we preferred to avoid it for the present purpose.

To determine the effect of the impurity bond on the entanglement entropy S between left side and right side, we performed extensive DMRG calculations. As usual in such calculations, we first determined the ground state wavefunction of (2) and then traced out the spin degrees of freedom of the right side to obtain the reduced density matrix ρ. The defect was inserted only at the last step of the procedure. We worked with $m = 500$ states and used no sweeps. The values of L varied between 3 and 401, corresponding to a total length of up to 801 sites. The computations were performed on the HPSC45 of ICTS, CAS.

To judge the accuracy of these calculations, we used the XX case, $\Delta = 0$, where the system becomes a simple free-fermion hopping model. Then one can determine ρ from the one-particle correlation function $C_{ij} =< c_i^\dagger c_j >$ by diagonalizing the matrix C in the subsystem [21]. Such calculations were done recently for segments in homogeneous chains with interface defects [18] and in random chains [22]. For the present geometry with open ends, this correlation function can be determined analytically for the pure system ($J_{imp} = 1$). Then one finds

$$C_{ij} = \frac{1}{4L}\left[\frac{\sin(\frac{\pi}{2}\frac{2L+1}{2L}(i-j))}{\sin(\frac{\pi}{4L}(i-j))} - \frac{\sin(\frac{\pi}{2}\frac{2L+1}{2L}(i+j))}{\sin(\frac{\pi}{4L}(i+j))}\right] \tag{4}$$

With a defect, C_{ij} has to be calculated numerically using the single-particle eigenfunctions of H and the filling. The corresponding results were considered as benchmarks. In Fig.1 we show the difference

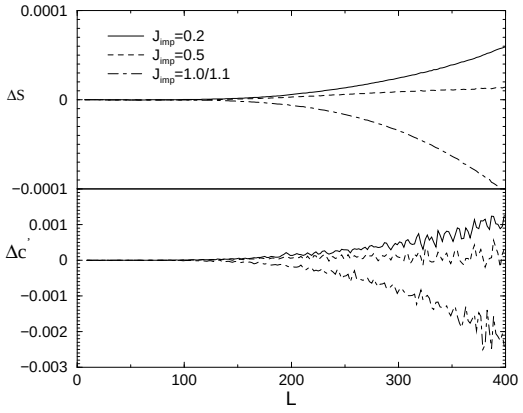

FIG. 1: Comparison between DMRG and correlation function results for the XX case and $J_{imp} = 0.2, 0.5$ and $1.0/1.1 = 0.9091$. Upper panel: Difference in the entanglement entropy S. Lower panel: Difference in the effective central charge c'.

between the DMRG results and the correlation function results for three defect strengths. Both ΔS and $\Delta c'$ increase with the chain length, as one would expect. From the upper panel one sees that the error in the entropy becomes about 10^{-4} for $L = 400$. The error in the effective central charge shown in the lower panel is larger and shows more noise. This is due to the numerical derivative by which one calculates c'

$$c'(L) = 6 \left[\frac{S(L+2) - S(L-2)}{\ln(L+2) - \ln(L-2)} \right] \tag{5}$$

and in which small differences enter. Thus $\Delta c'$ reaches about 10^{-3} at $L = 400$, which is still sufficient for our purposes. We expect the same accuracy also for the interacting system with Δ non-zero. Note that in (5) steps of 2 are used, because there still is a small even-odd oscillation in S. The two resulting values for c' approach each other for increasing L. In the following we always give results obtained for odd L.

II. SPECTRA

Before we present the results for the entanglement entropy we show some density-matrix spectra, since they determine the value of S. In Fig.2 spectra of the pure chain for fixed length and five different values of Δ are shown on the left. Plotted are the 100 largest eigenvalues w_n of ρ, ordered according to their magnitude. One sees the typical initial exponential decrease which then flattens out. A variation of Δ leads only to relatively small changes in the curves and S will also not be affected much. Note, however, that S is mainly determined by the first few large eigenvalues. On the right, the analogous spectrum is plotted for a defect with strength $J_{imp} = 0.5$. Here one can see a marked variation with Δ. The decay is fastest for $\Delta = -0.9$ and slowest for $\Delta = +0.9$. Because of the sum rule $\sum w_n = 1$, a slower decay is coupled with a smaller value for the first or first few eigenvalues [23]. This can be seen in the inset of the figure.

The size dependence of the spectra is shown in Fig.3 for two values of Δ. In both cases the curves become flatter as L increases, which is well-known from other DMRG calculations. The behaviour of the first eigenvalues, however, is different. For $\Delta = -0.9$ one has a region of relatively slow initial decay

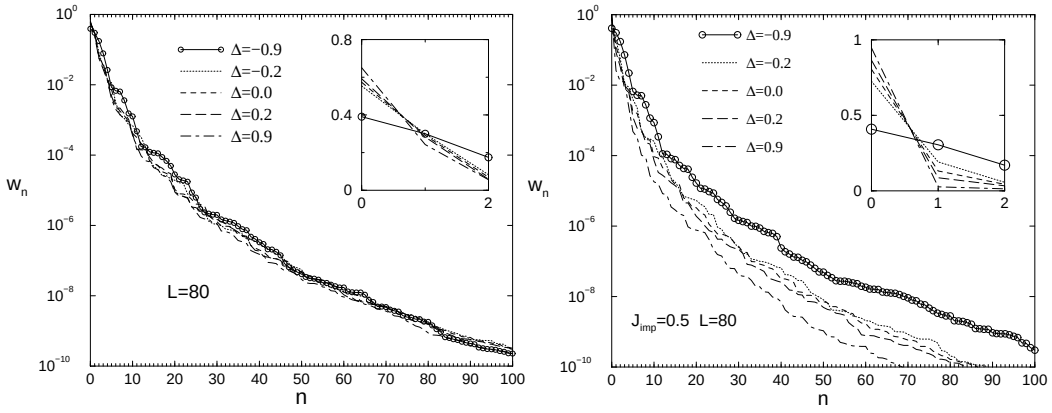

FIG. 2: Spectrum of the reduced density matrix for XXZ chains with various anisotropies. Left: pure chains. Right: defect strength $J_{imp} = 0.5$. Please note the logarithmic scale. The insets show the first three eigenvalues.

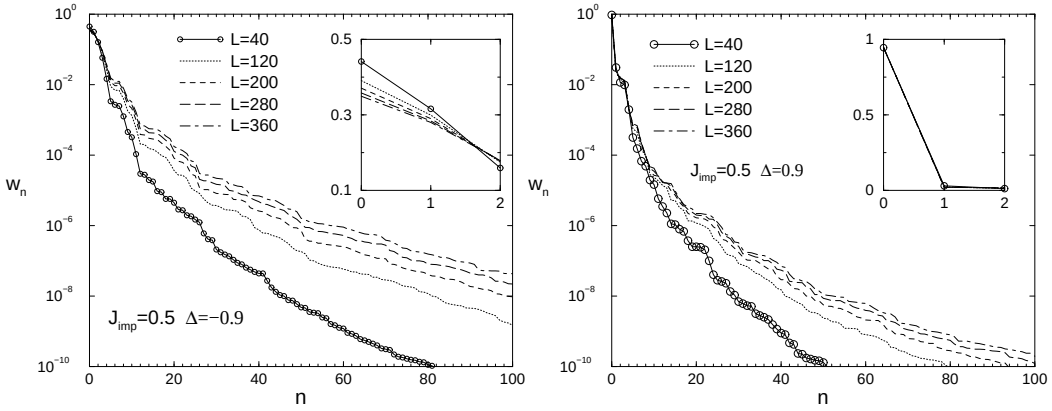

FIG. 3: Spectrum of the reduced density matrix for $J_{imp} = 0.5$ and various sizes L. Left: $\Delta = -0.9$. Right: $\Delta = +0.9$. The insets show the first three eigenvalues.

which becomes even slower as L increases. The first two eigenvalues decrease in accord with the remark made above. For S one therefore expects a relatively large value, because several w_n are of order 1, and a marked size dependence. For $\Delta = +0.9$, on the other hand, there is a gap between the first and the second eigenvalue and no visible change with L. Because of the rather fast decay of the complete spectrum, the sum rule is not effective here. Moreover, the largest eigenvalue w_0 is close to 1 and thus gives only a small contribution to S. Thus one expects a small absolute value and a weak size dependence of S here.

III. ENTANGLEMENT ENTROPY

Results for the entropy $S(L)$ are shown in Fig.4 for $J_{imp} = 0.5$ and sizes up to $L = 401$. One can see a monotonic increase with L for all values of Δ. The absolute value of S and the dependence on L are large for negative Δ and small for positive Δ, confirming the expectations based upon the spectra. The plot

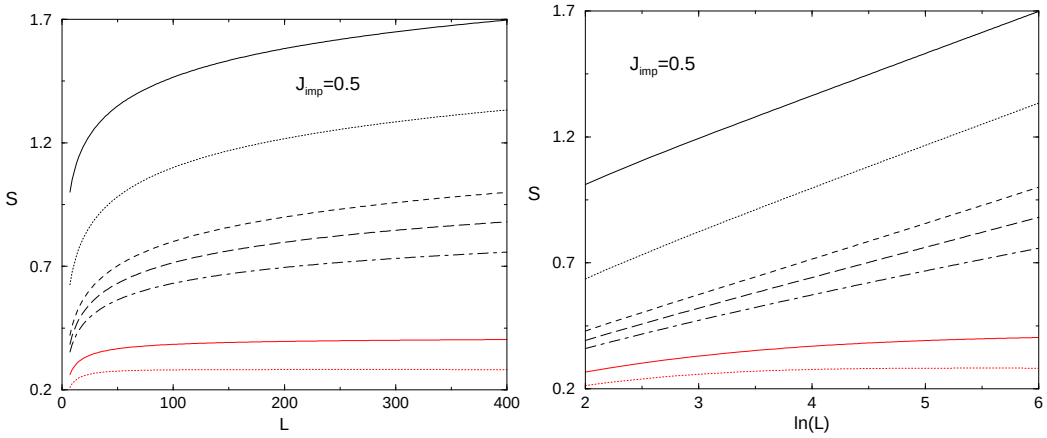

FIG. 4: Entanglement entropy as function of the system size for $J_{imp} = 0.5$ and seven values of the anisotropy. The data correspond to $\Delta = -0.9; -0.5; -0.1; 0; 0.1; 0.5; 0.9$, from top to bottom.

against $\ln L$ on the right hand side shows relatively straight curves with similar slopes in the first case but rather bent curves which seem to become horizontal in the second one. Thus there are characteristic differences between repulsive and attractive interactions. A determination of the slope and the effective central charge via (5) leads to the results shown in Fig. 5. The quantity c' clearly tends to the value 1 of the pure system for large negative Δ and to zero for large positive ones. The data for $\Delta = \pm 0.1$ also seem to fit into the pattern, while for $\Delta = 0$ the limit obviously differs from 1. This corresponds to the results in [18] where a continuous variation of the effective central charge with the defect strength was found in this case. For a detailed comparison, one has to take into account that the quantity c_{eff} used there referred to a subsystem coupled to the rest with e.g one modified and one unmodified bond. The contributions of these two bonds add up and the relation to c' is therefore

$$c_{eff}/3 = c'/6 + 1/6 \tag{6}$$

In [18] the asymptotic value of c_{eff} was determined by an extrapolation in $1/L$. The same procedure also works here and the results agree to 3-4 decimal places. In view of the rather different geometries in the two cases, this is a non-trivial consistency check of the calculations.

The right part of Fig.5 gives c' as a function of Δ and shows the different behaviour for positive and negative values very clearly. To show how these effects vary with the impurity strength, we present results for two other values of J_{imp}. In Fig. 6 this is done for a weaker bond, corresponding to a stronger perturbation. Then c' for the non-interacting case is only about 0.25 and even smaller for repulsion. For weak attraction, the values rise only slowly but for strong attraction they exceed 1 and approach it from above.

In Fig.7, on the other hand, the results for an only slightly weakened bond, $J_{imp} = 1/1.1 = 0.9090..$, are shown. In this case, not only the c' values for negative Δ lie rather close to 1, but also those for $\Delta = 0, 0.1$. Only for the larger Δ one has a reduction below 1, but the values are still rather high. From the left figure one sees that the curves for these Δ bend downwards and presumably approach zero for longer chains. However, the asymptotic region is beyond the range of our system sizes.

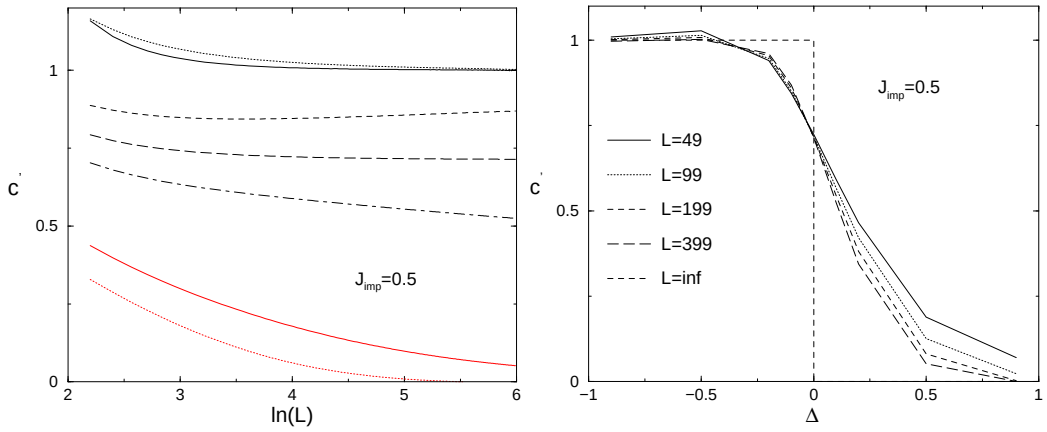

FIG. 5: Effective central charge for $J_{imp} = 0.5$. Left: as function of the system size for $\Delta = -0.5; -0.9; -0.1; 0; 0.1; 0.5; 0.9$, from top to bottom. Right: as function of the anisotropy.

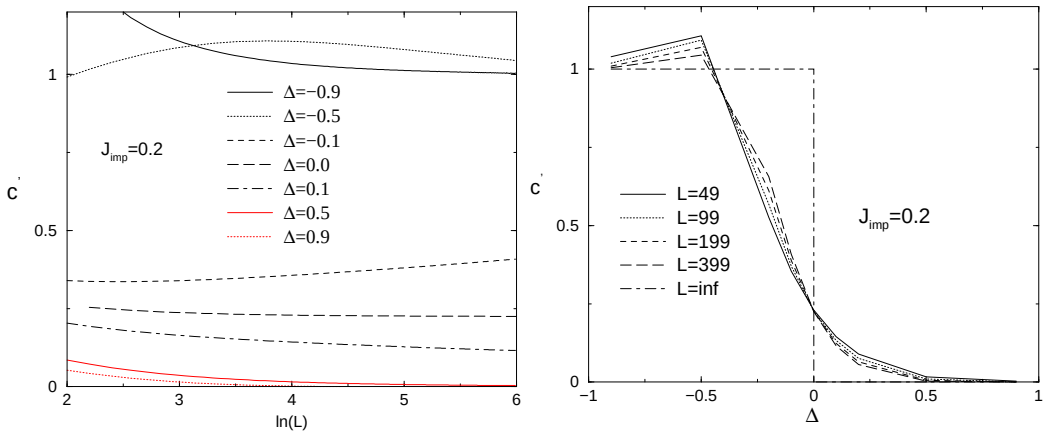

FIG. 6: The same as Fig. 5, but for $J_{imp} = 0.2$.

IV. DISCUSSION

These results show a clear distinction between attractive and repulsive interactions and a crossover between the two which is determined by the strength of the perturbation. This strength fixes the value of c' in the non-interacting system. Because this value depends only weakly on the size, it serves as a reference point through which the $c' vs. \Delta$ curves for different sizes go. The curves, which we determined only at a number of points, will be continuous in all finite systems. These findings are in line with the general predictions on the influence of an impurity in a Luttinger liquid, namely that for attraction the perturbation heals with increasing system size, while for repulsion it becomes stronger. For the weakened bonds which we have considered, the latter case means a scaling towards zero and a cutting of the chain. The vanishing of c' is in agreement with this picture, but the cutting should not be taken too literally since it only refers to processes near the Fermi energy. As Fig.4 shows, there remains a residual entanglement corresponding to the constant k in (1) which depends on the interaction strength.

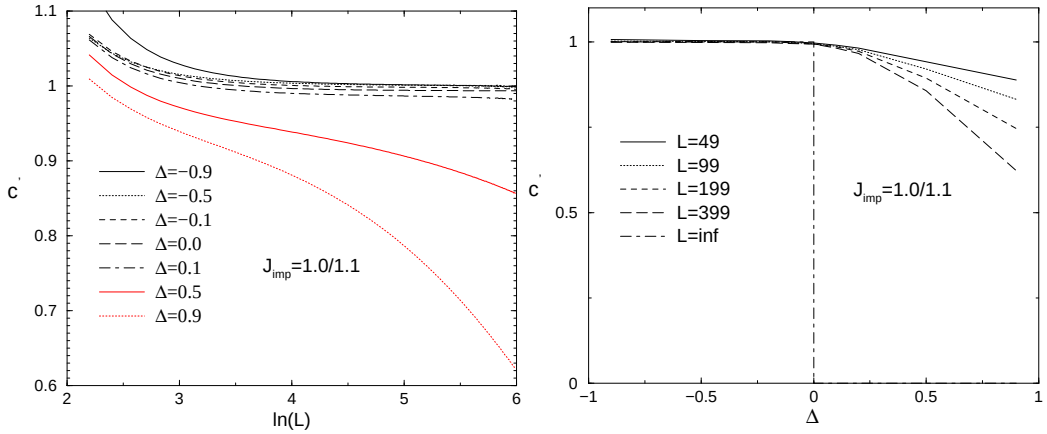

FIG. 7: The same as Fig. 5, but for $J_{imp} = 1/1.1 = 0.9091$. Please note the different vertical scale in the left figure.

There is no general expression for S in a finite system, not even for the XX case, but in [4] a formula was given for a weak impurity in a Luttiger liquid. The contribution to S is then

$$\delta S = -y^2\epsilon^2 \, \frac{g}{1-g^2} \, (\frac{L}{\epsilon})^{1-g} \ln(\frac{L}{\epsilon}) - b(g) \tag{7}$$

where y is the strength of the impurity potential, ϵ a small-distance cutoff, $b(g)$ a positive constant and g the Luttinger liquid parameter measuring the interaction. For the XXZ lattice model, it can be expressed as

$$\frac{1}{g} = 2\,(1 - \frac{1}{\pi}\arccos\Delta) \tag{8}$$

For attraction ($\Delta < 0$) one has $g > 1$ and for repulsion $g < 1$. In the latter case, δS is always negative and diverges with L. The numerical results for δS on the left of Fig.8 actually show this behaviour. One can also fit the data to equ.(7) as is shown on the right for $\Delta = 0.5$. The value of g is then 0.75 and the fit gives $\epsilon = 13$ and $b = 0.06$. However, similar fits for $\Delta = 0.1$ and 0.9 lead to very different results for ϵ and if one interprets it as an effective length determined by the scaling equations there are still inconsistencies. For attraction the L-dependent term in (7) is positive and decreases with L but the data for δS are more or less L-independent and cannot be fitted with reasonable parameters. Thus we cannot verify Levine's formula in detail. One should mention that he also predicts a $\ln^2 L$ term in δS for the non-interacting system which one does not see in the numerics. It could be that he used a too simple geometry for the two-dimensional bosonic field theory in his approach.

Summing up, we have shown by numerical calculations that the general effects of an impurity in a Luttinger liquid also show up in the entanglement entropy. Its logarithmic behaviour remains for attraction but is suppressed for repulsion. A more detailed analytical treatment is, however, still desirable.

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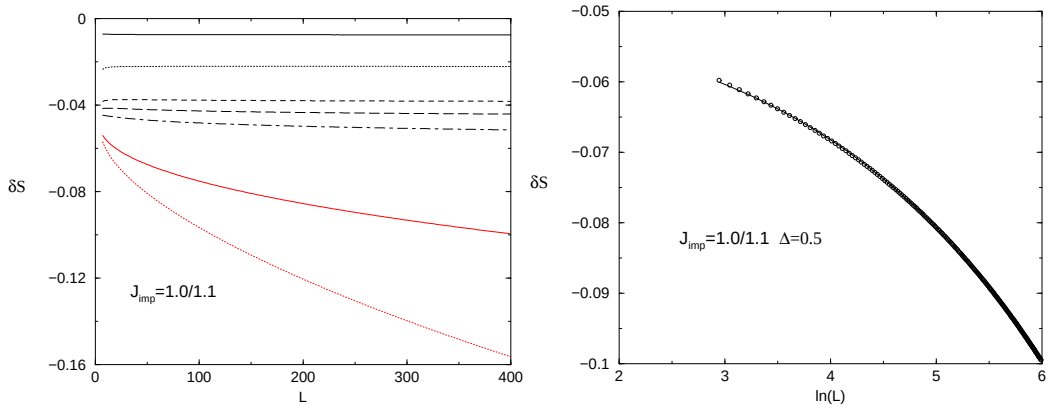

FIG. 8: Defect contribution δS to the entanglement entropy for $J_{imp} = 1/1.1$. Left: δS as function of L for $\Delta = -0.9; -0.5; -0.1; 0; 0.1; 0.5; 0.9$, from top to bottom. Right: Fit of the data (circles) for $\Delta = 0.5$ according to eqn.(7), see text.

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