Journal of Statistical Mechanics: Theory and Experiment
An IOP and SISSA journal

Fluctuations in subsystems of the zero-temperature XX chain: emergence of an effective temperature

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Received 21 September 2006
Accepted 7 November 2006
Published 24 November 2006

Online at stacks.iop.org/JSTAT/2006/P11013
doi:10.1088/1742-5468/2006/11/P11013

Abstract. The zero-temperature XX chain is studied with emphasis on the properties of a block of L spins inside the chain. We investigate the quantum fluctuations resulting from the entanglement of the block with the rest of the chain using analytical as well as numerical (density matrix renormalization group) methods. It is found that the rest of the chain acts as a thermal environment and an effective temperature can be introduced to describe the fluctuations. We show that the effective temperature description is robust in the sense that several independent definitions (through the fluctuation dissipation theorem, comparing with a finite temperature system) yield the same functional form in the limit of large block size ($L \to \infty$). The effective temperature can also be shown to satisfy the basic requirements on how it changes when two bodies of equal or unequal temperatures are brought into contact.

Keywords: spin chains, ladders and planes (theory), density matrix renormalization group calculations, entanglement in extended quantum systems (theory)

ArXiv ePrint: cond-mat/0609682

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Contents

1. Introduction

Entanglement properties of various spin chains have attracted much attention recently. The most intensively investigated cases are spin chains in their zero-temperature ground states, where the entanglement between a contiguous block of spins and the rest of the chain is measured through the von Neumann entropy. Thus far, the entanglement entropy has been found to be a well behaving measure of entanglement which shows some universal features at quantum critical points [1]–[5]. Despite capturing some important aspects, one should not forget that we inevitably lose information on the entangled state by using only a coarse grained measure. Indeed, the restriction of the pure ground state to a subsystem results in a mixed state with quantum fluctuations, and the weights are given by the full spectrum of the reduced density matrix, which means a number of parameters proportional to the exponential of the system size. Hence an 'integrated' measure such as the entropy will not tell us about the distribution of the fluctuations. This gives an obvious motivation for a deeper analysis of reduced density matrix spectra.

In the past few years, much effort has been devoted to the investigation of reduced density matrices in a series of simple model systems [6]–[10]. The results obtained indicate that, in several cases, the density matrix itself can be expressed as the exponential of a quadratic Hamiltonian. An example is the case for free fermions in one dimension (equivalent to an XX chain) which was investigated in detail [11]–[13] and the reduced density matrix for arbitrary subsystem sizes has been obtained in a closed form.

Here we try to develop a simple interpretation of the above results, concentrating on the XX chain. Looking at a subsystem of L spins in an infinitely large chain, the quantum fluctuations in the block are due to the coupling with the rest of the chain. One could think of an analogy with the subsystem–reservoir scheme of the canonical

doi:10.1088/1742-5468/2006/11/P11013

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ensemble in statistical physics where now the spins outside the block would play the role of the reservoir. Therefore it is an intriguing question whether it is possible to define an 'effective temperature' to describe the zero-temperature quantum fluctuations with Boltzmann-like distributions, meaning that the weights of the reduced density matrix $\hat{\rho}_L$ decay exponentially with the subsystem energies:

$$\hat{\rho}_L = \frac{1}{Z} \mathrm{e}^{-\beta_{\mathrm{eff}} \hat{H}_L}, \tag{1}$$

where $\hat{H}_L$ represents the Hamiltonian of the subsystem, and β_{eff} denotes the effective inverse temperature. The aim of this paper is to show that there are several ways to define an effective (inverse) temperature but they are all consistent in the sense that the leading order dependences on the subsystem size are identical, given by

$$\beta_{\mathrm{eff}} J = \pi \frac{L}{\ln L}, \tag{2}$$

where J is the coupling between nearest-neighbour spins. In the following we shall present a detailed derivation of the above result as outlined below.

In section 2, we give a brief summary of the results on the reduced density matrix of the XX chain [11]. Next (section 3), we analyse the one-particle spectra of the effective Hamiltonian emerging in the formula of the density matrix and that of the Hamiltonian describing a finite XX chain. We define the effective temperature starting out from a continuum limit formula for the eigenvalues [13], then verify these results by analysing the multiparticle spectra of finite systems either by means of the operator-based truncation scheme [12] or density matrix renormalization group (DMRG) calculations [14].

Section 4 is concerned with an alternative definition of the effective temperature, using an extension of the fluctuation dissipation theorem to zero temperature. The calculations are carried through for two different conserved quantities and the results obtained show agreement with the previous definitions.

With the concept of a system in an effectively thermodynamic environment, we try a direct mapping in section 5. The effective temperature is determined numerically by comparing canonical and zero-temperature expectation values. Surprisingly, we recover the results of the fluctuation dissipation ratio with a very high precision, and an explanation for the precise agreement is also given.

The definitions are also tested by studying their consistency with thermodynamics (section 6). Namely, we ask what happens when subsystems of equal or different temperatures are brought into contact. We find that equal temperatures do not change, while in case of unequal temperatures the resulting temperature is in between the initial ones.

Finally, we summarize our results (section 7) emphasizing also the problematic points which might set a limit on the applicability of the simple picture described here.

2. Reduced density matrix for the XX chain

Our starting point for the calculations is the Hamiltonian of the XX chain

$$\hat{H}^{XX} = -J \sum_{j=1}^{N-1} (s_j^x s_{j+1}^x + s_j^y s_{j+1}^y) - h \sum_{j=1}^{N} s_j^z, \tag{3}$$

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where s_j^α ($\alpha = x, y, z$) are the Pauli spin matrices at sites $j = 1, 2, \ldots, N$ of the chain, J is the coupling and h is the magnetic field. All our results, unless stated otherwise, are derived in the case of zero magnetic field ($h = 0$). It is well known that this model can be transformed into a chain of free fermions [15] with Hamiltonian

$$\hat{H} = -\tfrac{1}{2}\sum_{j=1}^{N-1}(c_j^\dagger c_{j+1} + c_{j+1}^\dagger c_j), \tag{4}$$

where $c_j^\dagger$ and c_j are fermionic creation and annihilation operators and energy is measured in units of the coupling J.

If one considers only a subsystem of size L in a large chain with N spins, the state of the subsystem is fully described by its reduced density matrix $\rho_L = \mathrm{tr}_{N-L}|\Psi_0\rangle\langle\Psi_0|$, obtained from the ground state $|\Psi_0\rangle$ by tracing out external degrees of freedom. It was previously shown [11] that for a chain with Hamiltonian (4) the reduced density matrix can be written in an exponential form

$$\hat{\rho}_L = \frac{1}{\tilde{Z}}\mathrm{e}^{-\tilde{H}}, \tag{5}$$

where $\tilde{Z} = \mathrm{Tr}(\mathrm{e}^{-\tilde{H}})$ is a normalization constant and $\tilde{H}$ is an effective Hamiltonian of the following form:

$$\tilde{H} = \sum_{i,j} A_{ij} c_i^\dagger c_j. \tag{6}$$

One can see that $\tilde{H}$ is quadratic in the fermionic operators. The matrix elements A_{ij} can be given through the elements of the correlation matrix $C_{ij} = \langle c_i^\dagger c_j\rangle$ by the following relation:

$$A = \ln\frac{1-C}{C}, \tag{7}$$

where A and C denote the matrices composed of the elements A_{ij} and C_{ij}, respectively. Hence, the effective Hamiltonian can be diagonalized, and the eigenvalues can be obtained through the eigenvalues ξ_k of the correlation matrix:

$$\tilde{H} = \sum_{k=1}^{L}\varepsilon_k f_k^\dagger f_k\,, \quad \varepsilon_k = \ln\frac{1-\xi_k}{\xi_k}, \tag{8}$$

where $f_k^\dagger$ and f_k are fermionic operators obtained by unitary transformation.

The diagonalization of the correlation matrix is especially simple if we take the whole system to be infinitely large ($N \to \infty$). In this case the elements of the matrix depend only on the distance $r = |i - j|$ between the sites and can be written as

$$C_{ij} = \frac{\sin((\pi/2)(i-j))}{\pi(i-j)} = \begin{cases} \dfrac{(-1)^{(r-1)/2}}{\pi r}, & r \text{ odd} \\ 0, & r \text{ even} \\ \frac{1}{2}, & r = 0. \end{cases} \tag{9}$$

For finite N, each element of the correlation matrix has to be evaluated numerically as a sum of N terms.

doi:10.1088/1742-5468/2006/11/P11013

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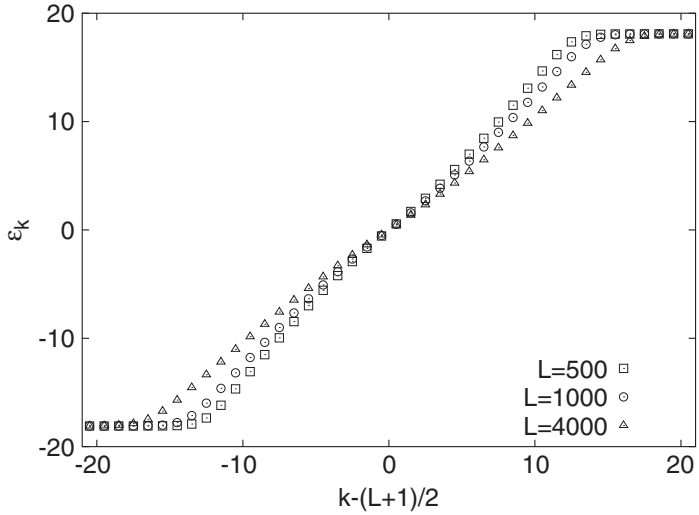

Figure 1. One-particle spectra of the effective Hamiltonian $\tilde{H}$ for various block sizes L with the chain size N taken to be infinite. The spectrum is shifted for each L to visualize the particle–hole symmetry. The saturation of the curves for $|k-(L+1)/2| > 10$ is due to numerical errors.

The purpose of studying the structure of the reduced density matrix $\hat{\rho}_L$ came from our intention to define an effective temperature by making a correspondence between the density matrix weights and Boltzmann factors (1) with respect to the subsystem Hamiltonian $\hat{H}_L$. This latter can be diagonalized exactly and it also transforms to a system of non-interacting fermions:

$$\hat{H}_L = \sum_{k=1}^{L} \lambda_k c_k^\dagger c_k \,, \quad \lambda_k = -\cos\left(\frac{\pi k}{L+1}\right). \tag{10}$$

Peschel's results show that $\hat{\rho}_L$ can be written as an exponential of a free fermion Hamiltonian (8). Thus, from comparison with (10) it can be seen that all the information we need is stored in the one-particle spectra ε_k and λ_k, where the former has to be numerically calculated.

3. One-particle and multiparticle spectra

Figure 1 shows the one-particle spectra of the effective Hamiltonian $\tilde{H}$ for various subsystem sizes with the chain size N taken to be infinite. First of all, we should notice the apparent particle–hole symmetry of the spectra, which is made more visible by shifting the curves to a common origin. This symmetry property is not surprising as it is already present in the spectrum of the XX chain with zero magnetic field. The saturation of the curves for $|k-(L+1)/2| > 10$ is due to numerical errors, since the major part of the eigenvalues of the correlation matrix C_{ij} lie exponentially close to 0 and 1.

The weights of the density matrix can be produced from these one-particle spectra in the same way as in the case of a real excitation spectrum: the largest weight is obtained by filling the modes up to the Fermi level, i.e. all modes that are negative. The next

largest weights are obtained by filling the smallest positive ε_k ('particle excitation') or removing the smallest negative one ('hole excitation'). Thus, the problem of finding the 2^L weights of the density matrix can be reduced to the diagonalization of an $L \times L$ matrix.

3.1. Continuum limit

Taking a continuum limit in the block ($L \to \infty$) Peschel calculated analytically the lowest lying eigenvalues [13]:

$$\varepsilon_j = \pm \frac{\pi^2}{2 \ln L}(2j-1), \qquad j = 1, 2, \ldots. \tag{11}$$

One can see that the spectrum is linear near the Fermi level and the eigenvalues scale with $1/\ln L$. Looking at the excitation spectrum of the block XX Hamiltonian $\hat{H}_L$, one finds that it is also linear near the Fermi level and, for large block sizes, it can be approximated as

$$\lambda_{k=L/2+j} = -\cos\left(\frac{\pi}{2} + \frac{\pi}{2}\frac{2j-1}{L+1}\right) \approx \frac{\pi}{2L}(2j-1). \tag{12}$$

Hence, the effective inverse temperature can be obtained by comparing only the low lying part of the one-particle spectra. From equations (11) and (12) one has

$$\beta_{\text{eff}} = \pi \frac{L}{\ln L}. \tag{13}$$

It can be seen that, according to the expectations, $\beta_{\text{eff}} \to \infty$ when $L \to \infty$; that is, we recover the zero-temperature ground state if we take the whole chain as the subsystem. It has to be emphasized that the above definition of the effective inverse temperature describes correctly only the low energy part of the spectrum. However, it is well known from DMRG calculations that, indeed, it is only a small portion of the weights which are relevant for the physics of the system [14], and therefore we also expect the effective temperature to be reasonably defined.

We should note that, comparing with numerical results, one finds deviations from the asymptotic formula (13). In the paper of Cheong and Henley [12], where the idea of defining an effective temperature first appeared, the logarithmic scaling of the eigenvalues could not be detected for system sizes $L < 100$; hence they found that $\beta_{\text{eff}} \propto L$. This can be understood since the logarithmic dependence on the block size makes convergence very slow and one needs corrections even for large block sizes ($L = 2000$–5000). Determining β_{eff} as the ratio of the lowest eigenvalues of (11) and (12) we have tried a fit $a \times L/(\ln L + b)$ which gave values $a = 3.12 \approx \pi$ and $b = 2.58$ which shows considerable finite size corrections, already noted in [13].

3.2. Operator-based truncation and DMRG results

In order to compare the results of the continuum limit for the effective temperature (13) to the one defined in equation (1), one has to consider finite size systems and build the multiparticle spectra from the one-particle spectra. A possible method is the so-called operator-based truncation scheme which was devised by Cheong and Henley [12] and consists of truncating the one-particle spectrum by retaining only a small number of the

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excitations symmetrically around the Fermi level. The method can be applied successfully, since the normalization constant $\tilde{Z}$ itself can be determined by using only the retained eigenvalues. Indeed, it can be verified [12] that

$$\frac{1}{\tilde{Z}} = \det(1 - C) = \prod_{k=1}^{L} \frac{1}{1 + \mathrm{e}^{-\varepsilon_k}}. \tag{14}$$

For large positive eigenvalues $1 + \mathrm{e}^{-\varepsilon_k} \approx 1$ while for large negative ones $1 + \mathrm{e}^{-\varepsilon_k} \approx \mathrm{e}^{-\varepsilon_k}$ and thus the latter terms simply cancel the factors of the occupied one-particle states in the exponential (5). Hence the most relevant weights of the reduced density matrix can be reproduced from the low lying excitations of the one-particle spectrum and the highly excited states, corrupted by numerical error, can be discarded.

The same method can be applied to obtain the multiparticle energy eigenvalues of the block, except that in this case we can calculate the given subset of the spectrum exactly, since the one-particle energies are known analytically. With this systematic procedure a one-to-one correspondence between the block energies and the density matrix weights can be established.

The multiparticle spectra constructed from the one-particle spectra have also been confirmed by the DMRG method [14]. In the DMRG method, the finite system is divided into two subsystems; thus the multiparticle spectra $\omega_\alpha(L)$ of the reduced subsystem density matrix and the eigenvalues $E_\alpha(L)$ of the reduced subsystem Hamiltonian can be calculated directly for a block of L spins, where α runs from one to the number of basis states, M, used to describe the block. We have calculated $\omega_\alpha(L)$ and $E_\alpha(L)$ as a function of the subsystem size L on finite chains with N lattice sites with open boundary condition using the dynamic block state selection (DBSS) approach [16]. The DBSS method allows a more rigorous control of the numerical accuracy by setting the threshold value of the quantum information loss χ and the minimum number of basis states, $M_{\min}$, used to describe the subsystem blocks prior to the calculations. For a given finite system with N lattice sites, subsystem blocks with $L = 2, \ldots, N-2$ can be obtained using the sweeping procedure of the so called finite lattice algorithm.

First, we have compared exact results obtained by exact diagonalization for $L = N/2$ on a short $N = 20$ chain to the DMRG results by systematically adjusting χ. In figure 2 we plotted $\omega_\alpha(L)$ as a function of $E_\alpha(L)$ obtained after the sixth DMRG sweep for various χ values with $M_{\min} = 16$. The accuracy of the diagonalization of the superblock Hamiltonian was set to 10^{-9}. The agreement between the exact diagonalization and DMRG results is evident from the figure for large $\omega_\alpha(L)$ even for large χ values. On the other hand, for the small $\omega_\alpha(L)$ spectrum more accurate calculations with smaller χ values have to be performed for better agreement.

In order to determine the size dependence of the effective temperature, similar calculations were repeated first for subsystems with $L = N/2$ by varying N and then by keeping the size of the system fixed but varying the size of the block. For the former case figure 3 shows our results for $N = 50, 100, 200, 400, 800$ using DMRG method with six sweeps, $\chi = 10^{-8}$, $M_{\min} = 1024$ and the operator-based truncation method with 20 particle–hole excitations kept. For large $\omega_\alpha(L)$ eigenvalues the agreement between the operator-based truncation and DMRG result is evident from the figure, while for the lower part of the spectrum the deviation between the two approaches due to truncation

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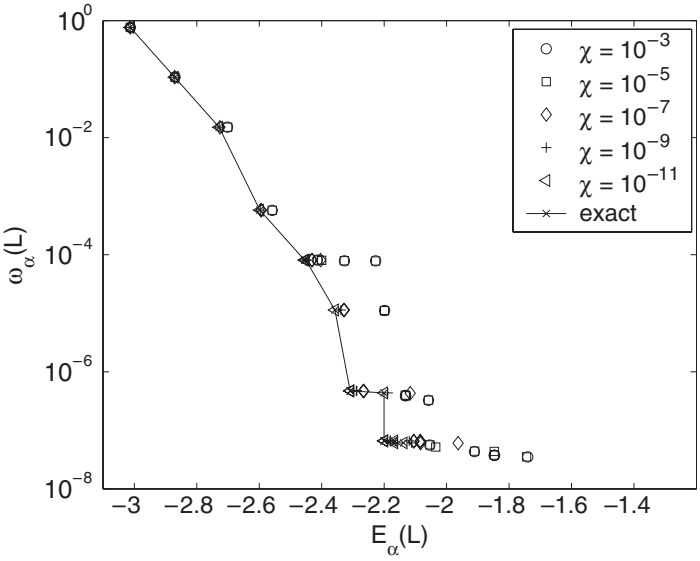

Figure 2. Eigenvalue spectrum of $\hat{\rho}_L$ as a function of the eigenvalues of $\hat{H}_L$ with $L = 10$ for a chain with $N = 20$ lattice sites for various χ values. The result of the exact diagonalization is shown by the solid line.

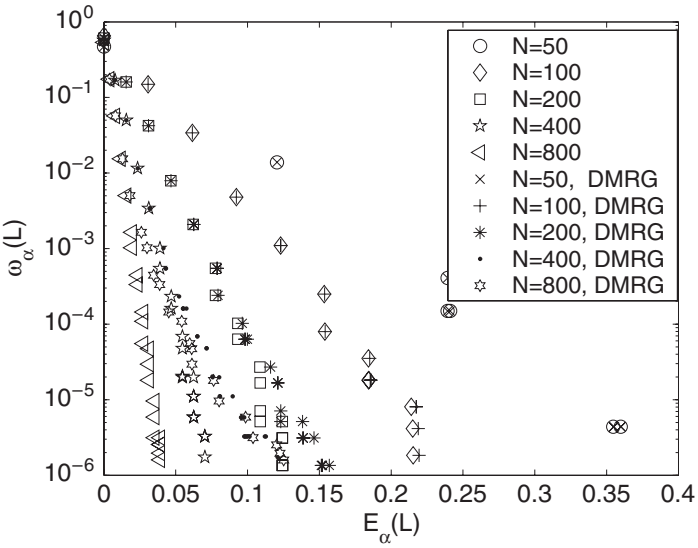

Figure 3. Eigenvalue spectrum of $\hat{\rho}_L$ as a function of the eigenvalues of $\hat{H}_L$ with $L = N/2$ for $N = 50, 100, 200, 400, 800$ using the operator-based truncation method and the DMRG algorithm with six sweeps. Degeneracies in the spectra are removed and all $E_\alpha(L)$ are measured from zero.

procedures is more significant. This result, however, confirms the validity of the operator-based truncation method and it is sufficient for determining the effective temperature. Data points corresponding to $\omega_\alpha(L) > 10^{-4}$ eigenvalues for each L can be fitted with a straight line in order to obtain $\beta_{\rm eff}(L)$ which is shown in figure 4. Our result indicates

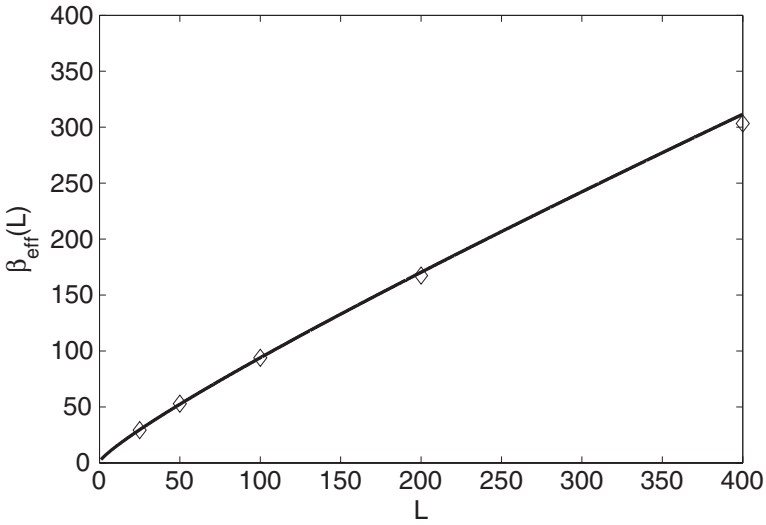

Figure 4. $\beta_{\rm eff}(L)$ as function of $L = N/2$ obtained as the absolute value of the slopes of straight line fits to the $\ln(\omega_\alpha(L))$ versus $E_\alpha(L)$ data sets. The solid line is the result of the fit with $a = 6.309$ and $b = 2.101$.

that $\beta_{\rm eff}(L)$ can be fitted in leading order with the ansatz $a \times L/(\ln L + b)$ and we obtained $6.42 > a > 5.76$ and $2.12 > b > 1.57$ depending on the number of data points taken into account when $\beta_{\rm eff}(L)$ was fitted by the straight lines. Using the operator-based truncation approach we repeated the same calculations with $L = N/4$ for $N = 200, 400, 800, 1600, 3200$ and found again that a changed between 6.37 and 5.63. The value of a close to 2π is twice that of given in equation (13). This is due to the fact that the blocks were always determined for a semi-infinite system having one open boundary. When the same calculations are carried out for chains with up to $N = 200$ lattice sites using DMRG with periodic boundary condition (PBC), in which case there are two couplings across the block interface, we obtained $3.3 > a > 2.9$ and $2.1 > b > 1.8$ in agreement with equation (13).

We have also calculated $\omega_\alpha(L)$ and $E_\alpha(L)$ for various finite chains with $N = 50, 100, 200, 400$ lattice sites for DMRG blocks with $L = 2, \ldots, N/2$ using several sweeps of the finite lattice algorithm. For a given N taking data set corresponding to $\omega_\alpha(L) > 10^{-4}$ a linear fit for each L can be obtained in order to determine $\beta_{\rm eff}(L)$ as a function of L. Our result shown in the left panel of figure 5 indicates that in leading order $\beta_{\rm eff}(L)$ can again be fitted very well with the following ansatz $a \times L/(\ln L + b)$. For all fits we obtained $6.38 > a > 6.21$ and b changed between 2.08 and 2.49. We also found that these fits are more stable than the above described previous approach. The value of a is again very close to 2π. When the same calculation is repeated using PBC we found $3.28 > a > 2.94$ and $2.12 > b > 1.81$ in agreement with equation (13) as also shown in the right panel of figure 5. The factor of two in a for OBC and PBC is the same effect as has been discussed for the entropy profile of a finite subsystem for critical models with open or periodic boundary conditions [4]. Finally, we conclude that a straight line fit is not enough to describe $\beta_{\rm eff}(L)$ as a function of L, but logarithmic corrections still could not be confirmed rigorously due to the limited system sizes.

doi:10.1088/1742-5468/2006/11/P11013

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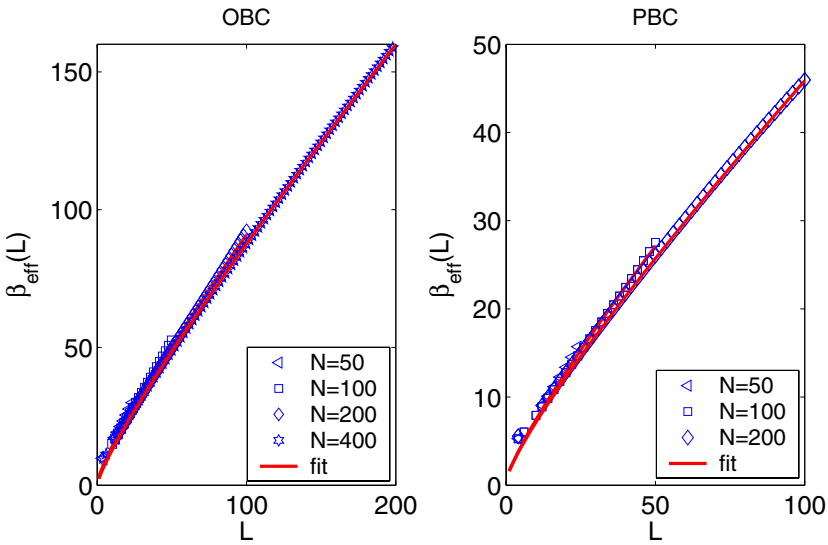

Figure 5. $\beta_{\rm eff}(L)$ as function of L obtained as the absolute value of the slopes of straight line fits to the $\ln(\omega_\alpha(L))$ versus $E_\alpha(L)$ data sets corresponding to finite chains with $N = 50, 100, 200, 400$ lattice sites. DMRG results, shown in the left and right panels, were obtained with open and periodic boundary conditions, respectively. The solid lines are the results of the fitting.

4. Fluctuation dissipation ratio

To support the idea of an effectively thermodynamic system, it would be desirable to find some alternative way of defining a temperature, and to compare the results of the different approaches. In ordinary thermodynamic systems, coupled to a reservoir at some finite temperature, the fluctuation dissipation theorem gives a possible way of defining the temperature. If we restrict ourselves to the static limit and consider only conserved quantities of the Hamiltonian, it reads

$$\chi_A = \beta(\langle \hat{A}^2 \rangle_\beta - \langle \hat{A} \rangle_\beta^2), \tag{15}$$

where $\hat{A}$ is a conserved quantity, and $\chi_A = \partial \langle \hat{A} \rangle_\beta / \partial h_A$ is the response function of $\hat{A}$ for an infinitesimal conjugate field h_A. The brackets denote averages taken with the canonical ensemble.

The straightforward generalization to our case would be to define the effective inverse temperature as the ratio of the response function to the fluctuations inside the block. We shall present here the calculations for two cases, using the transverse magnetization or the magnetization flux as the observable $\hat{A}$. From now on we shall consider only the case when the chain size N is taken to be infinite.

4.1. Fluctuations of the transverse magnetization

The transverse magnetization is a conserved quantity in the XX model, and thus it is a good candidate for the definition of the effective temperature, as described above:

$$\beta_{\rm eff} = \frac{\chi_M}{\langle \hat{M}_L^2 \rangle - \langle \hat{M}_L \rangle^2}, \tag{16}$$

where χ_M is the magnetic susceptibility, $\hat{M}_L$ is the transverse magnetization of the block, and the brackets now denote averages taken with $\hat{\rho}_L$. It is important to observe that we do not need the reduced density matrix to evaluate the expectation values since it is equivalent to calculating them in the ground state $|\Psi_0\rangle$ of the whole chain, which is known exactly.

Let us begin by calculating the block magnetization in the case of an applied magnetic field. The ground state $|\Psi_h\rangle$ is known exactly [15], and we have

$$\langle\Psi_h|\hat{M}_L|\Psi_h\rangle = \sum_{j=1}^{L}\left\langle c_j^\dagger c_j - \frac{1}{2}\right\rangle = \frac{L}{2\pi}\int_{-\pi}^{\pi}\langle c_q^\dagger c_q\rangle \mathrm{d}q - \frac{L}{2} = L\left(\frac{q_h}{\pi} - \frac{1}{2}\right), \tag{17}$$

where $q_h = \arccos(-h)$ is the Fermi wavenumber. The magnetic susceptibility is therefore

$$\chi_M = \left.\frac{\partial\langle\hat{M}_L\rangle}{\partial h}\right|_{h=0} = \frac{L}{\pi}. \tag{18}$$

The fluctuations in (16) have to be evaluated at $h = 0$, when the block magnetization $\langle\hat{M}_L\rangle$ is vanishing, and hence the fluctuations read

$$\langle\hat{M}_L^2\rangle = \sum_{i,j=l}^{L}\langle s_i^z s_j^z\rangle = \sum_{i,j=1}^{L}\langle c_i^\dagger c_i c_j^\dagger c_j\rangle - \frac{L^2}{4}. \tag{19}$$

Using Wick's theorem and introducing the difference $r = i - j$ of the sites we obtain

$$\langle\hat{M}_L^2\rangle = -2\sum_{i<j=2}^{L} C_{ij}^2 + \frac{L}{4} = -\frac{2}{\pi^2}\sum_{\substack{r=1\\ r\,\mathrm{odd}}}^{L-1}\frac{L-r}{r^2} + \frac{L}{4}, \tag{20}$$

where the elements of the correlation matrix C_{ij} were given in equation (9). It is easy to see that the linear terms in L cancel, and the asymptotic form of the fluctuations will be

$$\langle\hat{M}_L^2\rangle \approx \frac{1}{\pi^2}(\ln L + c), \quad c = \ln 2 + \gamma + 1. \tag{21}$$

Note that (21) is consistent with a result in [17] where the leading order size dependence of the particle number fluctuations has been obtained in case of free gapless fermions in arbitrary dimensions. Therefore the effective inverse temperature is obtained as

$$\beta_{\mathrm{eff}} = \pi\frac{L}{\ln L + c}, \tag{22}$$

which is a form very similar to (13); however there is a correction to the logarithm already seen at the numerical evaluation of the one-particle spectra.

4.2. Fluctuations of the magnetization current

To further verify the validity of our description, we shall calculate the fluctuation dissipation ratio for another conserved quantity, the magnetization current. When the

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whole system is in equilibrium, the expectation value of the current flowing through the subsystem is vanishing, though there are still current fluctuations inside the block, which can be calculated using the equilibrium ground state.

However, in order to obtain the response function, one needs to drive the system out of equilibrium. Therefore we need the ground state of the chain with a magnetization flux, a problem which has been solved by Antal *et al* in [18]. We briefly summarize the method leading to the main results and refer the reader to [18] for the details.

First, one needs to calculate the current density

$$\hat{j}_l = s_l^y s_{l+1}^x - s_l^x s_{l+1}^y = \frac{1}{2\mathrm{i}}(c_l^\dagger c_{l+1} - c_{l+1}^\dagger c_l), \tag{23}$$

and then introduce a modified Hamiltonian $\hat{H}^M = \hat{H} - \lambda \hat{J}$ with the Lagrange multiplier λ, where $\hat{J} = \sum_l \hat{j}_l$. Note that λ will now play the role of the conjugate field of the magnetization current.

The ground state of the above modified Hamiltonian will give us a current carrying steady state of the XX chain with a prescribed amount of current. Since $[\hat{H}, \hat{J}] = 0$, Hamiltonian $\hat{H}^M$ can be diagonalized exactly and the resulting one-particle spectrum has the following form ($h = 0$):

$$\Lambda_q = -\frac{1}{\cos\varphi}\cos(q - \varphi), \tag{24}$$

with $\varphi = \arctan(\lambda)$. One can see that the spectrum is just the original XX spectrum shifted by the wavenumber φ, and rescaled by $\cos\varphi$. Having obtained the structure of the ground state $|\Psi_\lambda\rangle$, the elements of the correlation matrix can be evaluated and yield

$$\langle\Psi_\lambda|c_l^\dagger c_m|\Psi_\lambda\rangle = g(m-l) = \begin{cases} \dfrac{(-1)^{(r-1)/2}}{\pi r}\mathrm{e}^{\mathrm{i}r\varphi}, & r \text{ odd}, \\ 0, & r \text{ even}, \\ \frac{1}{2}, & r = 0, \end{cases} \qquad r = m - l. \tag{25}$$

We are interested in the response function of the block for an infinitesimal change in the conjugate field λ. The expectation value of the magnetization current has to be evaluated in the current carrying ground state:

$$\langle\Psi_\lambda|\hat{J}_L|\Psi_\lambda\rangle = \frac{1}{2\mathrm{i}}\sum_{l=1}^{L-1}(g(1) - g^*(1)) = \frac{L-1}{\pi}\sin\varphi = \frac{L-1}{\pi}\frac{\lambda}{\sqrt{1+\lambda^2}}, \tag{26}$$

and hence the response function is given by

$$\left.\frac{\partial\langle\hat{J}_L\rangle}{\partial\lambda}\right|_{\lambda=0} = \frac{L-1}{\pi}, \tag{27}$$

which, for large values of L, is the same as the magnetic susceptibility (18).

Next, the current fluctuations have to be calculated in equilibrium. With $\langle\hat{J}_L\rangle = 0$, we need only

$$\langle\hat{J}_L^2\rangle = -\tfrac{1}{4}\sum_{l,m=1}^{L-1}\langle(c_l^\dagger c_{l+1} - c_{l+1}^\dagger c_l)(c_m^\dagger c_{m+1} - c_{m+1}^\dagger c_m)\rangle. \tag{28}$$

Using Wick's theorem, the contribution from terms with $|m-l|>1$ is

$$-\tfrac{1}{2}\sum_{|m-l|>1}\left[|g(m-l)|^2-\mathrm{Re}\,(g(m-l+1)g^*(m-l-1))\right], \tag{29}$$

while the $|m-l|=0,1$ terms give

$$\frac{L-1}{2}\left[g(0)(1-g(0))+\frac{g^2(1)+g^2(-1)}{2}\right]-(L-2)|g(1)|^2. \tag{30}$$

Introducing $r=m-l$ and using the equilibrium value of the matrix elements $g(r)$, the fluctuations read

$$\langle\hat{J}_L^2\rangle=\frac{L-1}{2}\left(\frac{1}{4}+\frac{1}{\pi^2}\right)-\frac{1}{\pi^2}\left(\sum_{r\,\mathrm{even}}^{L-2}\frac{L-1-r}{r^2-1}+\sum_{r\,\mathrm{odd}}^{L-1}\frac{L-1-r}{r^2}\right). \tag{31}$$

The asymptotics of the above expression can be given as

$$\langle\hat{J}_L^2\rangle\approx\frac{1}{\pi^2}(\ln L+c'),\qquad c'=\ln 2+\gamma+1/2, \tag{32}$$

which differs slightly from (21) in the next to leading order term. Looking at equations (27) and (32) we recover again the same leading order size dependence of β_{eff}.

To conclude, we emphasize that the results obtained for the effective temperatures coincide in leading order. This is important since now contributions from all of the excited states are included in definition (16), while the theoretical construction in section 3 used only the lowest lying states.

5. Mapping to a thermalized system

In the previous section we defined the effective temperature starting out from the fluctuation dissipation theorem, which is known to be valid for real thermodynamic systems at finite temperature. The idea behind our approach is a possible mapping of the subsystem in the infinite chain at $T=0$ to a finite system which is thermalized at some finite temperature.

A more direct way of testing this mapping would be to compare expectation values in both of the above mentioned settings. That is, one has to consider an XX chain of finite length L connected to a heat bath, and try to adjust the temperature in such a way that the expectation value of a given quantity would be exactly the same as in the entangled block at zero temperature.

Since the total transverse magnetization $\hat{M}$ of the finite chain is vanishing at any temperature for $h=0$, we shall choose the fluctuations to compare. Thus, the effective inverse temperature β^* is defined from the equality

$$\langle\hat{M}^2\rangle_{\beta^*}=\langle\hat{M}_L^2\rangle, \tag{33}$$

where the subscript on the bracket denotes an expectation value taken in the canonical ensemble with an inverse temperature β^*, while the right-hand side is the $T=0$ fluctuation. We changed the notation for the effective inverse temperature to avoid confusion with the former definition (16). The rhs of the equation was already determined in (20); thus one has to evaluate only the canonical expectation value.

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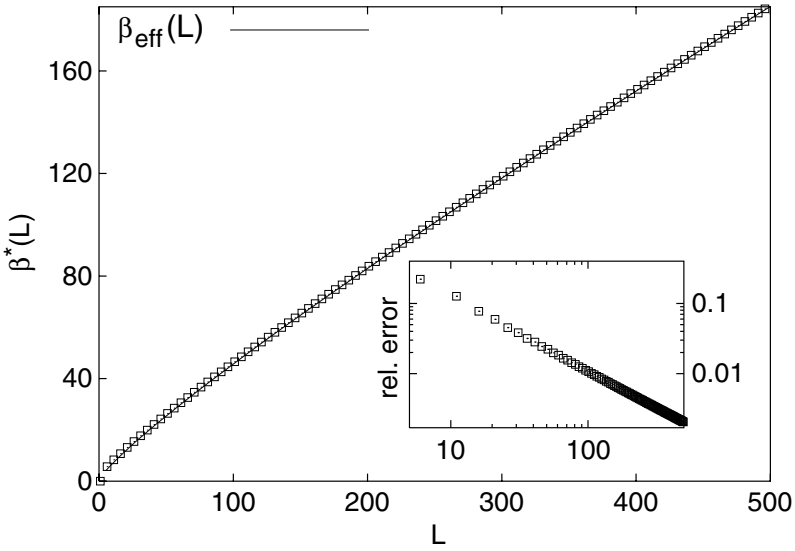

Figure 6. Effective inverse temperature obtained by solving equation (33) numerically (squares). The solid line represents the asymptotic value, equation (22), obtained from the fluctuation dissipation relation at zero temperature. The inset shows the relative deviation from the asymptotic curve.

First we calculate the partition function $Z = \mathrm{Tr}(\mathrm{e}^{-\beta \hat{H}_L})$. Since the XX Hamiltonian can be transformed into a set of non-interacting fermions, the partition function can be evaluated exactly for arbitrary values of the magnetic field:

$$Z(\beta, h) = \prod_{k=1}^{L} (1 + \mathrm{e}^{-\beta \lambda_k}), \tag{34}$$

where $\lambda_k = -\cos(\pi k/(L+1)) - h$ is the one-particle spectrum of $\hat{H}_L$.

Starting out from the partition function one can calculate the moments of the magnetization as logarithmic derivatives with respect to the magnetic field. The expectation value reads

$$\langle \hat{M} \rangle_\beta = \frac{1}{\beta} \frac{\partial \ln Z}{\partial h} - \frac{L}{2} = -\frac{1}{2} \sum_{k=1}^{L} \tanh\left(\frac{\beta \lambda_k}{2}\right), \tag{35}$$

while the fluctuations can be obtained as

$$\langle \hat{M}^2 \rangle_\beta - \langle \hat{M} \rangle_\beta^2 = \frac{1}{\beta^2} \frac{\partial^2 \ln Z}{\partial h^2} = \frac{1}{4} \sum_{k=1}^{L} \frac{1}{\cosh^2(\beta \lambda_k/2)}. \tag{36}$$

We have now a closed form for either side of the equation (33); therefore β^* can be calculated numerically for arbitrary system sizes. Figure 6 shows the results of the calculations together with the asymptotic form obtained from the fluctuation dissipation ratio. Apparently, either definition for the effective temperature gives the same result, and the deviation (see the inset) from the asymptotic curve tends to be relatively small even for moderate system sizes.

doi:10.1088/1742-5468/2006/11/P11013

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The precise agreement of the inverse temperatures might look surprising, but it has a simple explanation in the given case. Namely it is the consequence of the temperature independent susceptibility. Indeed, looking at the formula of the magnetization (35), one has a sum of tangent hyperbolic terms, a function which is known to saturate for large arguments. For large system sizes β^* is expected to be large; thus the non-trivial terms in the sum are those where $\lambda_k \approx 0$, that is the Fermi level of the spectrum. However, as already shown in (12), the spectrum is linear near the Fermi level; thus application of a small field will cause a shift in the spectrum, nevertheless preserving linearity. Hence, the terms in the sum near the Fermi level cancel, the tangent hyperbolic being an odd function, and the result depends only on the difference in the number of terms added on the saturated tails. This is of course determined by the shift alone that is independent of temperature.

Now, if the susceptibility is temperature independent and we use the definition (16) of the effective temperature, the following relation holds:

$$\beta^* \langle \hat{M}^2 \rangle_{\beta^*} = \beta_{\text{eff}} \langle \hat{M}_L^2 \rangle, \tag{37}$$

which, together with (33), results in $\beta^* = \beta_{\text{eff}}$; that is, the different definitions are identical.

6. Subsystems in contact

When one speaks about the temperature of a system there are some basic properties the definition has to fulfil. For example, when we take two systems with equal temperatures and place them in contact, the resulting system must have the same temperature as the initial ones.

A possible analogue of this situation in our case is the following. We take two semi-infinite chains with blocks of length L on the boundaries and join them together. The resulting block of length $2L$ in the infinite chain has to have an effective temperature dictated by equation (22).

In order to solve this problem, we shall calculate the effective inverse temperature for a block of L spins at the boundary of a semi-infinite chain using again the fluctuation dissipation approach for the transverse magnetization. Following the steps of section 4.1 we shall first calculate the magnetization with a non-zero magnetic field:

$$\langle \hat{M}_L \rangle = \sum_{j=1}^{L} \frac{2}{\pi} \int_0^{q_h} \mathrm{d}q \sin^2(qj) - \frac{L}{2} = L\left(\frac{q_h}{\pi} - \frac{1}{2}\right) - \frac{1}{\pi} \sum_{j=1}^{L} \frac{\sin(2jq_h)}{2j}, \tag{38}$$

where now brackets denote averages taken in the ground state of the semi-infinite chain.

One can see that the first term of the above result coincides with the one obtained for the infinite chain (17); however the second term has an explicit dependence on the location of the block sites which is the consequence of broken translational symmetry. Taking the derivative at zero magnetic field, the second term becomes zero for even and $-1/\pi$ for odd L; thus for even L we recover the infinite chain result (18) exactly.

For the fluctuations we need the elements of the correlation matrix C_{ij}^s of the semi-infinite chain which can be given as

$$C_{ij}^s = \frac{\sin((\pi/2)(i-j))}{\pi(i-j)} - \frac{\sin((\pi/2)(i+j))}{\pi(i+j)}. \tag{39}$$

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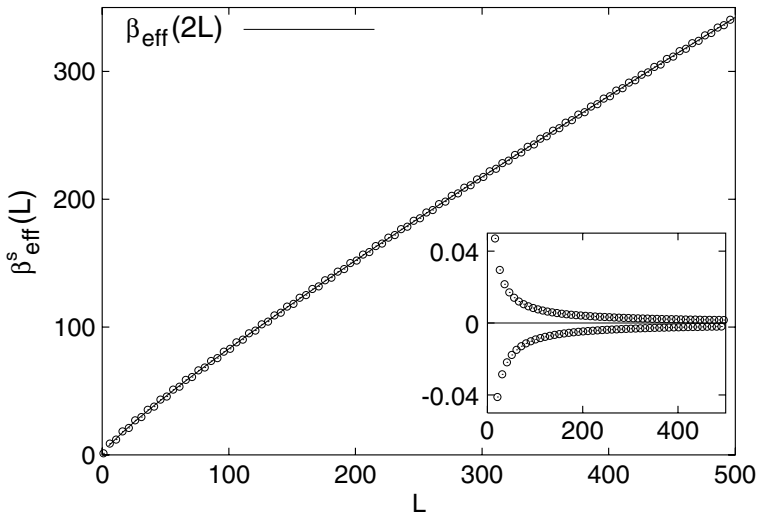

Figure 7. Effective inverse temperature of a block of $2L$ spins in an infinite chain (solid line) and a block of L spins on the boundary of a semi-infinite chain (circles). The inset shows the relative deviation from the $\beta_{\rm eff}(2L)$ line. The oscillations are due to the difference between even/odd block sizes.

Now, one has to simply substitute C_{ij} with C^s_{ij} in equation (20). Introducing the difference $r = i - j$ and the sum $s = i + j$ of the sites we have

$$\langle M_L^2 \rangle = -\frac{2}{\pi^2} \sum_{\substack{r=1 \\ r\,\text{odd}}}^{L-1} \sum_{\substack{s=2+r \\ s\,\text{odd}}}^{2L-r} \left[\frac{1}{r^2} + \frac{1}{s^2} + 2\frac{(-1)^{(r+s)/2}}{rs} \right] + \frac{L}{4}. \tag{40}$$

We were able to evaluate the above sum only numerically. The result for the effective inverse temperature $\beta^s_{\rm eff}(L)$ of a block of L spins in the semi-infinite chain is shown in figure 7 together with the effective inverse temperature $\beta_{\rm eff}(2L)$ of a block of size $2L$ in an infinite chain. One can see an excellent agreement between the two results along with oscillations which might originate from the difference between even and odd block sizes. It is reasonable to think that these oscillations might be interpreted through the fact that the interaction between the spins generates anticorrelations between the transverse spin components; thus all quantities whose definition involves transverse correlations (such as the effective temperature) will be sensitive to the parity of the system size.

In addition to verifying that the effective temperature does not change when bringing two subsystems of the same size into contact, we also obtained the formula

$$\beta^s_{\rm eff} = 2\pi \frac{L}{\ln L + \ln 2 + c}, \tag{41}$$

which is valid when the block is at the boundary of a semi-infinite chain, and c is the constant defined in (21). This result also confirms the factors close to 2π instead of π, obtained when fitting to the DMRG results with open boundary conditions.

With the formula (41) in hand, we can also confirm another thermodynamic property of the temperature. Namely, if we take two subsystems of different temperatures and bring them into contact the resulting temperature of the joint system must have a temperature

between the two initial values. Changing to effective inverse temperatures, this means that the following inequalities should hold:

$$\beta^s_{\rm eff}(L) < \beta_{\rm eff}(L+L') < \beta^s_{\rm eff}(L'), \qquad \text{if } L < L'. \tag{42}$$

In order to prove (42), we use the equality $\beta^s_{\rm eff}(L) = \beta_{\rm eff}(2L)$ and require the positivity of the derivative of $\beta_{\rm eff}(L+L')$ respect to L and L'. This requirement yields the condition $\ln(L+L') + c > 1$. As one can see, this condition holds even for the smallest possible unequal system sizes ($L = 1$, $L' = 2$) provided $c > 0$ which is what we have found in all our calculations.

7. Final remarks

We have presented an effective thermodynamic description of an entangled block in an XX spin chain at zero temperature. For a better understanding of the range of validity of this picture several comments are in order.

First of all, it has to be noted that during our investigation of the one-particle spectrum of the effective Hamiltonian (8), we dealt only with the eigenvalues and did not look at the appropriate eigenstates. It was already demonstrated in [13] that, in contrast to the homogeneous plane wave eigenstates of the open XX chain, the eigenstates of the embedded block show enhanced amplitudes near the boundaries. Nevertheless, all those states with symmetrically occupied particle–hole excitations, such as the ground state, are identical. Furthermore, certain quantities such as the transverse magnetization have the same expectation values in either of the one-particle states. However, it is clear that the role of this strange amplitude enhancement requires deeper understanding, especially when dealing with quantities that are sensitive to boundary effects. It is possible that in such cases the validity of this simple thermodynamic picture might be lost, or at least requires more careful considerations.

It would be also desirable to test the fluctuation dissipation approach with some non-conserved quantity, e.g. the longitudinal magnetization. Unfortunately, in such cases the calculation of the response function is fairly involved, since the model becomes non-integrable when the appropriate field is switched on. Even so, there remains the possibility of determining the response function numerically by means of DMRG calculations for finite chains.

It is also reasonable to expect that the effective temperature description might be carried over to other simple conformally invariant models, such as the critical transverse Ising chain, where the form of the reduced density matrix of a subsystem is rather similar to that for the XX case [6, 10]; however the exact form of the effective temperature might be somewhat different.

One can also speculate on the effect of placing the system in a heat bath of finite inverse temperature $\beta_{\rm hb}$. It is reasonable to expect the effective temperature not to change dramatically as long as thermal fluctuations are subdominant of the quantum fluctuations, i.e. when $\beta_{\rm hb} \gg \beta_{\rm eff}$. On the other hand, when the temperature of the heat bath becomes much larger than the effective temperature ($\beta_{\rm hb} \ll \beta_{\rm eff}$), the subsystem should be thermalized by the heat bath. Therefore, the behaviour of a subsystem should change when the inverse temperature of the heat bath is on a scale $\beta_{\rm hb} \propto L/\ln L$. This condition has been actually found for the temperature of the transition between the logarithmic

doi:10.1088/1742-5468/2006/11/P11013

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and extensive behaviours of the entropy in gapless free fermionic systems [17], further supporting the existence of an effective temperature.

As far as higher dimensional systems are considered, we remark on an other result of [17] where the fluctuations of the transverse magnetization have been found to scale as $L^{d-1} \ln L$ with the system size in arbitrary dimensions. This property together with the extensive character of the susceptibility might lead us to speculate that our fluctuation dissipation approach would result in an effective temperature with a same dependence on the linear size also in higher dimensions. We emphasize, however, that these arguments require more careful investigations.

Finally, it should be pointed out that there is an opportunity for extending our calculations to non-equilibrium situations, such as the driven XX chain. We believe that the simple definitions that we applied in the equilibrium case could be easily carried over, and the results may shed light on the possibility of introducing an effective temperature in systems far from equilibrium.

Acknowledgments

We would like to thank Ingo Peschel for a stimulating discussion. This work was financially supported by OTKA Grants Nos T043734, TS044839, T043330 and F046356 and the János Bolyai Research Fund.

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