Density-matrix spectra for two-dimensional quantum systems

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For a two-dimensional system of coupled oscillators, the spectra of reduced density matrices can be obtained analytically. This provides an example where the features of these quantities, which are of central importance in numerical studies using the density-matrix renormalization-group method, can be seen.

The density-matrix renormalization-group (DMRG) method[1] has brought enormous progress to the study of one-dimensional quantum systems and related classical problems.[2] Consequently, this numerical approach has also been applied to two-dimensional quantum problems.[3,4] The situation there, however, appears to be much less favorable.

The reason for this has to be sought in the properties of the density matrices which are used to select an optimal reduced basis in the Hilbert space. The essential quantity is the distribution of their eigenvalues. In one dimension, one usually finds a rapid decay, so that a relatively small number of states is sufficient to give very good results. This basically exponential decay can be derived explicitly for noncritical integrable models.[5,6] In nonintegrable cases, the spectra are less regular, but still have similar features.[7,8]

The situation in two dimensions has been discussed in some detail for free fermions,[9] and for the transverse Ising model.[10] It was found that, if one couples one-dimensional chains to form ladders, the number m of states one needs to maintain a certain accuracy grows exponentially with the width M of the system. This was derived either from the limit of noninteracting chains, or from numerical calculations. The spectra themselves, however, have not been discussed so far, although they are at the core of the problem. It therefore seems worthwhile to treat an example, where one can give explicit results.

This is possible for a system of coupled harmonic oscillators, which is integrable in any number of dimensions. This problem was studied recently for the case of a linear chain,[6] and it was shown that the ground-state density matrices, either for one site or for half of the system, are exponentials of bosonic operators. This is a consequence of the Gaussian form of the ground state, and holds quite generally. The problem is only to determine the bosonic eigenvalues. This can be done either numerically for a small system, or analytically in the thermodynamic limit.

To be specific, consider the system described by the Hamiltonian

$$H=\sum_i \left(-\frac{1}{2}\frac{\partial^2}{\partial u_i^2}+\frac{1}{2}\omega_0^2 u_i^2\right)+\sum_{i,j}\frac{1}{2}k_{ij}(u_i-u_j)^2, \quad (1)$$

where u_i is the coordinate of the ith oscillator, and ω_0 its frequency. The masses are all equal to unity, and the oscillators are coupled by springs of strength k_{ij}. Transforming H to normal coordinates, one can write down the ground state immediately. In terms of the original coordinates, it has the form

$$\phi=\exp\left(-\frac{1}{2}\sum_{i,j} A_{ij}u_i u_j\right). \quad (2)$$

The total density matrix is then $|\phi\rangle\langle\phi|$. By integrating out part of the coordinates, one obtains reduced density matrices which have the diagonal form

$$\rho=C\exp\left(-\sum_j \varepsilon_j b_j^\dagger b_j\right), \quad (3)$$

with bosonic operators b_j and $b_j^\dagger$. The eigenvalues ε_j follow from a matrix which is obtained from A_{ij}, and has a dimension equal to the number of kept sites. One divides A_{ij} into four submatrices a^{11}, a^{12}, a^{21}, and a^{22}, according to whether the sites i and j are kept or not. Then the matrix $a^{11}[a^{12}(a^{22})^{-1}a^{21}]^{-1}$ has eigenvalues $\cosh^2(\varepsilon_j/2)$. This can be shown by a straightforward generalization of the approach in Sec. II of Ref. 6. In this way, density-matrix spectra can be calculated numerically for an arbitrary assembly of coupled oscillators.

For a large system, however, the situation simplifies. In Ref. 6 it was shown that, for a chain with nearest-neighbor coupling k and oscillator frequency $\omega_0=1-k$, ε_j, for half of the system, in the thermodynamic limit, are given by

$$\varepsilon_j=(2j-1)\varepsilon, \quad j=1,2,3,\ldots, \quad (4)$$

where

$$\varepsilon=\pi I(k')/I(k). \quad (5)$$

Here $I(k)$ is the complete elliptic integral of the first kind, and $k'=\sqrt{1-k^2}$. The result is also valid for finite systems if the size is large compared with the correlation length. ε_j for smaller systems are still similar, but there are deviations from Eq. (4) which increase for larger values of j.

Now consider a two-dimensional square lattice of oscillators with nearest-neighbor couplings k_x and k_y in the two directions. This can be reduced to a one-dimensional problem by first introducing normal coordinates in the columns. The corresponding normal frequencies are

$$\omega(q)^2=\omega_0^2+2k_y(1-\cos q), \quad (6)$$

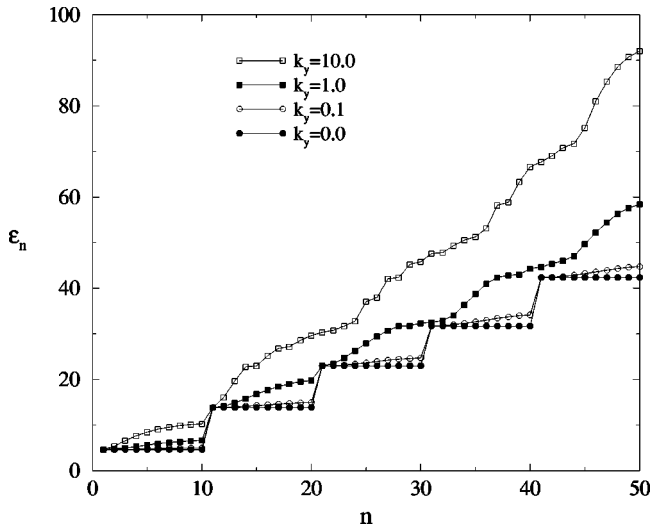

FIG. 1. Bosonic single-particle eigenvalues $\varepsilon_j(q)$, cf. Eq. (3), for half of a 10×10 system, arranged in ascending order, for $\omega_0 = k_x = 1.0$, and four values of the coupling k_y.

where the vertical momenta for open boundary conditions at the ends and M sites are given by

$$q = \frac{m}{M}\pi, \quad m = 0,1,2,\ldots,(M-1). \tag{7}$$

If one now couples the columns, the different momenta do not mix, and for each value of q a horizontal chain of the form of Eq. (1) results, where the oscillator frequency is now $\omega(q)$ and the coupling k_x. For the density matrix of the half-system, this leads to the spectrum of Eqs. (4) and (5), with the parameter $k = k(q)$ determined from the relation $k_x/\omega(q) = k/(1-k)$ or, explicitly,

$$k = k_x/[k_x + \omega(q)]. \tag{8}$$

In this way, an analytic expression for the spectrum is obtained. For each j, one has a band of M eigenvalues $\varepsilon_j(q)$ due to the transverse extension of the system. This reflects the corresponding interface between the two parts into which the system is divided. The dispersion of the vibrational modes in the vertical direction also determines the dispersion of the ε band via Eq. (8). In particular, a large $\omega(q)$ also leads to a large value of ε.

Such spectra, calculated numerically for a 10×10 lattice, are shown in Fig. 1. Plotted are $\varepsilon_j(q)$, arranged according to their magnitude for different values of the transverse coupling k_y. For noninteracting horizontal chains, one has a sequence of plateaus. Turning on $k_y(>0)$, the eigenvalues increase except for $q=0$ and form real bands. At the lower end, the stairlike structure still persists, while for larger values of j the bands are spread more due to the factor $(2j-1)$, and eventually overlap. After the proper ordering of the ε's, a continuous curve emerges. It corresponds roughly to a linear relation of the form

$$\varepsilon_n \cong \lambda n, \tag{9}$$

with an integer n, and $\lambda \cong 2\varepsilon(q=0)/M$ inversely proportional to the width M.

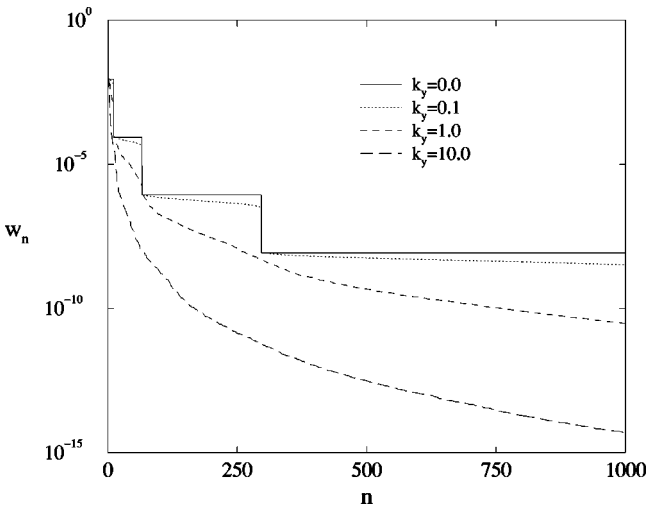

FIG. 2. Density-matrix eigenvalues w_n, arranged in decreasing order, obtained from $\varepsilon_j(q)$ in Fig. 1 and for the same parameters.

The actual eigenvalues w_n of ρ are obtained by specifying the occupation numbers of the bosonic single-particle levels $\varepsilon_j(q)$. This leads to an increasingly larger number of possibilities as more ε's are involved, i.e., for smaller w_n. The final result is shown in Fig. 2 for the same parameters as in Fig. 1. One can see that the stairlike structure also persists in w_n for small k_y, although the plateaus are much longer and given by combinatorical factors. For larger k_y, rather smooth curves arise which drop increasingly more quickly. In all cases, there is a rapid initial decay followed by a slower decrease for larger n. Following Ref. 7, one can derive an asymptotic formula from Eq. (9) which reads

$$w_n \sim \exp\{-[\lambda/(2\pi^2/3)]\ln^2 n\}, \tag{10}$$

and which is obeyed reasonably well by the curves. Due to the slow decay, the truncation error when cutting off the spectrum also decreases slowly. After $n=100$, 500, and 1000, it is approximately 10^{-5}, 10^{-7} and 10^{-8}, respectively, if $k_x = k_y = \omega_0 = 1.0$.

The dependence of the w_n spectrum on the width M is shown in Fig. 3 for the case $k_x = k_y = 1$. One can see how the

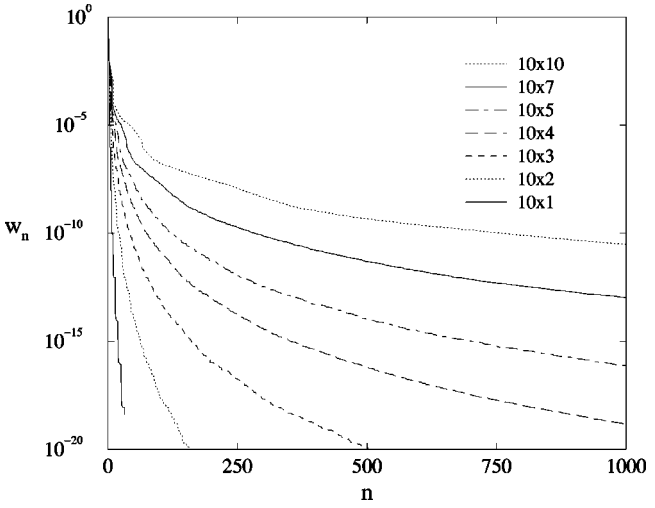

FIG. 3. Density-matrix eigenvalues w_n for systems of different width M and $\omega_0 = k_x = k_y = 1.0$.

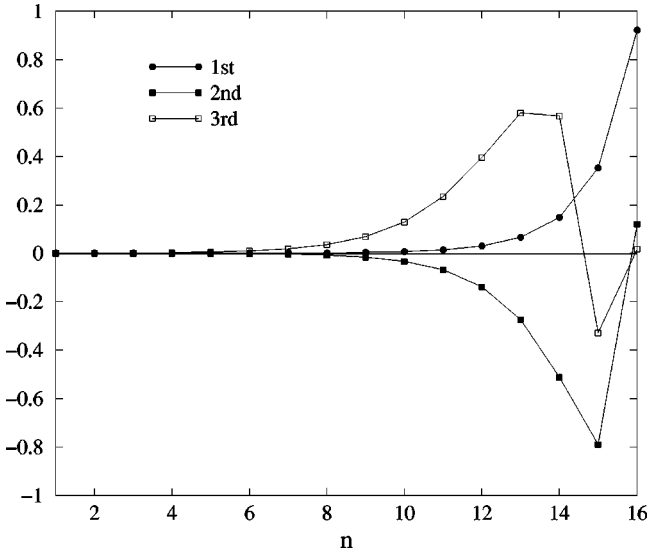

FIG. 4. Density-matrix eigenstates for the left part of a chain of 32 sites. Shown are the amplitudes as a function of the position for the lowest three ε_j values for $\omega_0 = k = 0.5$.

curves drop more and more slowly as M increases, in accordance with Eqs. (9) and (10) and the decrease of λ with M.

These results confirm that the situation worsens as the system becomes more two dimensional. The faster initial decay before the onset of the combinatorical effects helps in numerical calculations. Also, the interaction helps here to some extent, since the ε values increase with k_y, but this does not remove the basic $1/M$ dependence in the exponent. The same features are found if one assumes that one is dealing with fermionic operators in Eq. (3). This would correspond to a fermionic system with pair terms such that the Hamiltonian expressed in Fermi operators has the same structure as Eq. (1) expressed in Bose operators. In this case, the combinatorical possibilities are reduced, but this leads only to a change $\lambda \to 2\lambda$ in Eq. (10). One should also note that we have treated a noncritical system where the situation is in general more favorable. One could extend the considerations to three dimensions, in which case one has two momenta for the transverse directions, and therefore an even larger number of ε values in each band.

Returning briefly to one dimension, we would like to mention that our model also shows the origin of the different DMRG performance for chains and rings[1] very clearly. This problem is, in fact, closely related to those discussed above. If one calculates the density-matrix spectrum for a half-ring, one finds the same ε_j values at the lower end as for the half-chain, but each value appears *twice*. When plotted, this leads to a structure as in Fig. 1, with steps of length two. The reason lies in the form of the eigenstates of ρ which, for small ε_j, are concentrated near the boundary between system and environment. This feature, which was conjectured before,[1,11] can be seen explicitly here, and is illustrated in Fig. 4. The effect is known from the closely related corner transfer matrix of the massive Gaussian model.[12] For a half-ring, which has two points of contact, one then finds two such sets of states which are approximately independent of each other for small ε_j. Therefore, $\rho \cong \rho_L \rho_R$, where ρ_L and ρ_R are density matrices for only a left boundary or only a right boundary. Thus the situation is the same as for a ladder consisting of two only weakly interacting chains.

Coming back to the two-dimensional problem, the spectra found here explain, in a very direct way, the difficulties of the DMRG in this case. To apply the method, one should use as many symmetries as possible.[10] However, to treat very large systems, a procedure which avoids the extended interfaces between the parts of the system would be necessary. Whether the momentum-space approach of Ref. 4 can help here is not yet clear.

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