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 DMRG method, can be seen.

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

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 non-critical integrable models. In non-integrable cases, the spectra are less regular but still have similar features.

The situation in two dimensions has been discussed in some detail for free fermions and for the transverse Ising model. It was found that, if one couples one-dimensional chains to form ladders, the number of states one needs to maintain to get a certain accuracy, grows exponentially with the width of the system. This was derived either from the limit of non-interacting 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 worth while 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 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

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

where \( u_i \) is the coordinate of the i-th oscillator and \( \omega_0 \) 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

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

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

\[ \rho = C \exp \left( -\sum_j \varepsilon_j b_j^\dagger b_j \right) \]

with bosonic operators \( b_j, b_j^\dagger \). The eigenvalues \( \varepsilon_j \) 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 \( a_1^{11}, a_1^{12}, a_1^{21}, a_1^{22} \), according to whether the sites \( i \) and \( j \) are kept or not. Then the matrix \( a_1^{11}[a_1^{12}(a_1^{22})^{-1}a_1^{21}]^{-1} \) has eigenvalues \( \cosh^2(\varepsilon_j/2) \). This can be shown by a straightforward generalization of the approach in section 2 of [1].
way, density-matrix spectra can be calculated numerically for an arbitrary assembly of coupled oscillators.

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

\[
\varepsilon_j = (2j - 1)\varepsilon, \quad j = 1, 2, 3, \ldots \tag{4}
\]

where

\[
\varepsilon = \pi I(k')/I(k) \tag{5}
\]

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. The \( \varepsilon_j \) for smaller systems are still similar, but there are deviations from (5) which increase for larger values of \( j \).

Now consider a two-dimensional square lattice of oscillators with nearest-neighbour 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

\[
\omega(q) = \omega_0^2 + 2k_y(1 - \cos q) \tag{6}
\]

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

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

If one now couples the columns, the different momenta do not mix, and for each value of \( q \) a horizontal chain of the form (6) 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 (5, 6) 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 \( \varepsilon \)-band via (6). In particular, a large \( \omega(q) \) also leads to a large value of \( \varepsilon \).

Such spectra, calculated numerically for a 10×10 lattice, are shown in Fig. 1. Plotted are the \( \varepsilon_j(q) \) arranged according to their magnitude for different values of the transverse coupling \( k_y \). For non-interacting 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 stair-like structure still persists, while for larger values of \( j \) the bands are spread more due to the factor \( (2j - 1) \) and overlap eventually. After the proper ordering of the \( \varepsilon \), a continuous curve emerges. It corresponds roughly to a linear relation of the form

\[
\varepsilon_n \cong \lambda n \tag{9}
\]

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

The actual eigenvalues \( w_n \) of \( \rho \) 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 \( \varepsilon \) 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 stair-like structure persists also in the \( w_n \) 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 faster. In all cases, there is a rapid initial decay followed by a slower decrease for larger \( n \). Following [7], one can derive an asymptotic formula from (9) which reads

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

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 \( k_x = k_y = 1.0 \). One can see how the curves drop more and more slowly as \( M \) increases, in accordance with (9) and (10) and the decrease of \( \lambda \) 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 \( \varepsilon \)-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 [8]. This would correspond to a fermionic system with pair terms such that the Hamiltonian expressed in Fermi operators has the same structure as (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 (10). One should also note that we have treated a non-critical system where the situation is in general more favourable. 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 \( \varepsilon \)-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 \( \varepsilon_j \)-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 \( \rho \) which, for small \( \varepsilon_j \), 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 $\varepsilon_j$. Therefore, $\rho \equiv \rho_L \cdot \rho_R$ where $\rho_L$ and $\rho_R$ are density matrices for only a left or only a right boundary. Thus the situation is the same as for a ladder consisting of two only weakly interacting chains.

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{fig4}
\caption{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 $\varepsilon_j$-values for $\omega_0 = k = 0.5$.}
\end{figure}

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 really 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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