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LETTER TO THE EDITOR

Calculation of reduced density matrices from correlation functions

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Abstract

It is shown that for solvable fermionic and bosonic lattice systems, the reduced density matrices can be determined from the properties of the correlation functions. This provides the simplest way to these quantities which are used in the density-matrix renormalization group method.

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Reduced density matrices for solvable fermionic and bosonic lattice models have been studied in recent years because such operators play a central role in the density-matrix renormalization group (DMRG) method [1–3]. In contrast to the quantities used in other cases, they refer to a subset of *sites*, not to a subset of particles. It has been found that they have exponential form $e^{-\mathcal{H}}$, where \mathcal{H} is again a solvable fermionic or bosonic operator, confined to the chosen subsystem [4–6]. This was derived by starting from the total density matrix (usually for the ground state) and integrating the degrees of freedom outside the subsystem. In the case of fermions, this can be done using Grassmann variables. The procedure is straightforward, but also somewhat tedious. However, it was noted recently that for a hopping model the final result involves only the one-fermion correlation functions of the system [7]. In the following, it is shown that one can go a step further and base the considerations completely on correlation functions. The density matrices then follow in a very simple and transparent way.

Consider first a system of free fermions hopping between lattice sites. The corresponding Hamiltonian has the general form

$$\hat{H} = - \sum_{n,m} \hat{t}_{nm} c_n^\dagger c_m \quad (1)$$

where the ‘hat’ denotes quantities of the total system. This Hamiltonian has Slater determinants as eigenstates. Let $|\Psi\rangle$ be such a state and

$$\hat{C}_{nm} = \langle c_n^\dagger c_m \rangle \quad (2)$$

the one-particle function in this state. The \hat{C}_{nm} form a Hermitian matrix \hat{C} . Because $|\Psi\rangle$ is a determinant, all the higher correlation functions can be expressed by \hat{C} , e.g.

$$\langle c_n^\dagger c_m^\dagger c_k c_l \rangle = \langle c_n^\dagger c_l \rangle \langle c_m^\dagger c_k \rangle - \langle c_n^\dagger c_k \rangle \langle c_m^\dagger c_l \rangle. \quad (3)$$

Now consider a subsystem of M sites for which the notation i, j will be used. By definition, the reduced density matrix ρ reproduces all expectation values in the subsystem. Therefore, the one-particle function is

$$C_{ij} = \text{Tr}(\rho c_i^\dagger c_j) \quad (4)$$

and the higher functions must factorize as in (3). According to Wick's theorem, this property holds if ρ is the exponential of a free-fermion operator [8]. Thus one can write

$$\rho = \mathcal{K} e^{-\mathcal{H}} \quad (5)$$

where \mathcal{K} is a normalization constant and

$$\mathcal{H} = \sum_{i,j} H_{ij} c_i^\dagger c_j. \quad (6)$$

Let $\phi_k(i)$ be the eigenfunctions of H with eigenvalues ε_k . Then the transformation to new fermion operators a_k ,

$$c_i = \sum_k \phi_k(i) a_k \quad (7)$$

diagonalizes \mathcal{H} and ρ becomes

$$\rho = \mathcal{K} \exp\left(-\sum_{k=1}^M \varepsilon_k a_k^\dagger a_k\right). \quad (8)$$

Using this in (4) together with $\text{Tr}(\rho) = 1$ gives

$$C_{ij} = \sum_k \phi_k^*(i) \phi_k(j) \frac{1}{e^{\varepsilon_k} + 1}. \quad (9)$$

On the other hand, H has the representation

$$H_{ij} = \sum_k \phi_k(i) \phi_k^*(j) \varepsilon_k. \quad (10)$$

Therefore the eigenvalues ζ_k of C and ε_k of H are related by

$$\zeta_k = (e^{\varepsilon_k} + 1)^{-1} \quad (11)$$

and in matrix form, with the prime denoting the transpose,

$$H' = \ln[(1 - C)/C]. \quad (12)$$

This is the formula found in [7]. Due to its form, ρ is completely determined by the $M \times M$ matrix C . One should note that *any* one-particle correlation function can be expressed in such a way through a proper free-fermion operator. The only condition is that the eigenvalues ζ_k of C lie between 0 and 1 and this is always the case, since they can be written in the form $\langle a_k^\dagger a_k \rangle$ with new fermion operators [9]. However, for a state which is not a Slater determinant, the free-fermion density matrix found above would in general give wrong results for other expectation values.

These considerations can be extended to systems with pair creation and annihilation which can be diagonalized by a Bogoliubov transformation. The eigenstates are then Slater determinants in the new Fermi operators. In such a state, 'anomalous' correlation functions

$$\hat{F}_{nm} = \langle c_n^\dagger c_m^\dagger \rangle \quad (13)$$

exist which also occur in the factorization equations. Thus (3) is changed into

$$\langle c_n^\dagger c_m^\dagger c_k c_l \rangle = \langle c_n^\dagger c_l \rangle \langle c_m^\dagger c_k \rangle - \langle c_n^\dagger c_k \rangle \langle c_m^\dagger c_l \rangle + \langle c_n^\dagger c_m^\dagger \rangle \langle c_k c_l \rangle. \quad (14)$$

To reproduce this, ρ has to be an exponential with an operator \mathcal{H} which also contains pair creation and annihilation processes,

$$\mathcal{H} = \sum_{i,j} \left[c_i^\dagger A_{ij} c_j + \frac{1}{2} (c_i^\dagger B_{ij} c_j^\dagger + \text{h.c.}) \right]. \quad (15)$$

Since now two matrices appear in \mathcal{H} , one needs additional input, which is provided by the correlation functions F_{ij} . By following the usual diagonalization procedure for \mathcal{H} [10] and calculating C and F one can then show that

$$[(C - 1/2 - F)(C - 1/2 + F)]_{ij} = \frac{1}{4} \sum_k \phi_k(i) \phi_k^*(j) t h^2(\varepsilon_k/2) \quad (16)$$

where the $\phi_k(i)$ are the orthonormal eigenfunctions of $(A - B)(A + B)$ and the ε_k are again the single-particle eigenvalues of \mathcal{H} . Thus one can find the ε_k from the eigenvalues of the matrix on the left-hand side of (16). This matrix can be written as $K K^\dagger/4$ where $K/2 = (C - 1/2 - F)$, since F is anti-Hermitian. Having diagonalized $K K^\dagger$, the matrices A and B can be obtained as

$$A_{ij} = \frac{1}{2} \sum_k [\phi_k(i) \psi_k^*(j) + \psi_k(i) \phi_k^*(j)] \varepsilon_k \quad (17)$$

$$B_{ij} = -\frac{1}{2} \sum_k [\phi_k(i) \psi_k^*(j) - \psi_k(i) \phi_k^*(j)] \varepsilon_k \quad (18)$$

where the functions ψ_k follow from $t h(\varepsilon_k/2) \psi_k = -K^\dagger \phi_k$. For $F = 0$, one has $K = K^\dagger$, $\psi_k = \phi_k$ and therefore $B = 0$, while the result for A corresponds to (10). If one turns a hopping model into that with pair terms via a particle-hole transformation, (16) follows from (9). To make contact with the treatment in [6], one first relates the matrix \hat{G} , used there to write an even-parity eigenstate in the form

$$|\Psi\rangle = \mathcal{C} \exp \left\{ \frac{1}{2} \sum_{n,m} \hat{G}_{nm} c_n^\dagger c_m^\dagger \right\} |0\rangle \quad (19)$$

where $|0\rangle$ is the vacuum of the c_n , to the quantities appearing here. For the ground state, \hat{G} connects the two sets of functions $\hat{\phi}_p$ and $\hat{\psi}_p$ arising in the diagonalization of the Hamiltonian. The same holds for $\hat{K}/2 = (\hat{C} - 1/2 - \hat{F})$ and one finds that $\hat{G} = (\hat{K} - 1)/(\hat{K} + 1)$. Using this, one can show that the matrix in (A9) of [6] equals $2(1 + K K^\dagger)/(1 - K K^\dagger)$.¹ Therefore the eigenvalue equation used in [6] to determine $2ch\varepsilon_k$ is an alternative version of relation (16) and both approaches are fully consistent.

In a similar way, one can treat systems of coupled harmonic oscillators. In this case, it is convenient to consider the correlation functions of positions and momenta,

$$\hat{X}_{nm} = \langle x_n x_m \rangle \quad \hat{P}_{nm} = \langle p_n p_m \rangle. \quad (20)$$

In the ground state, which is a Gaussian in the coordinates, one then has factorization formulae such as

$$\langle x_n x_m x_k x_l \rangle = \langle x_n x_m \rangle \langle x_k x_l \rangle + \langle x_n x_k \rangle \langle x_m x_l \rangle + \langle x_n x_l \rangle \langle x_m x_k \rangle \quad (21)$$

which are non-trivial even if all indices are equal. They hold also if the expectation values are calculated with an exponential operator quadratic in the x and p . Therefore ρ has the form (5) with

$$\mathcal{H} = \frac{1}{2} \sum_{i,j} [T_{ij} p_i p_j + V_{ij} x_i x_j]. \quad (22)$$

¹ In [6], equation (15) has to read $\alpha = a^{11} - ca^{22}c'$ and $\alpha/2$ should appear in (16).

The diagonal form is again (8) but with bosonic operators and the ε_k follow from the eigenvalues v_k^2 of the matrix XP via

$$cth(\varepsilon_k/2) = v_k/2. \quad (23)$$

If the subsystem is a single oscillator i , there is only one v given by $\langle x_i^2 \rangle / \langle p_i^2 \rangle$. For a homogeneous system, this can also be expressed through the frequency moments of the normal modes as $\langle 1/\omega \rangle \langle \omega \rangle$. The general equations are again equivalent to those obtained previously in [5].

This shows that the way to reduced density matrices associated with eigenstates of solvable fermionic or bosonic systems can be shortened considerably. The results are also valid for systems at finite temperature as considered in [7]. In connection with the DMRG, the main aim has been to determine the spectra of the ρ and their general features. Here the present approach helps if the necessary correlation functions have simple analytic expressions. This is the case for nearest-neighbour hopping on a chain, or on a square lattice for half filling. Then only the diagonalization of the matrix C remains. There are some limitations, because if large ε_k occur, the corresponding eigenvalues of C are exponentially close to 0 or 1. Also the relation of ρ to the corner transfer matrix of a two-dimensional model [4, 11] is not visible unless one determines \mathcal{H} in its non-diagonal form. Still, one comes rather close to an analytical solution, and working with the correlations can give additional insight into the nature of the problem.

Note added. Formulae similar to those given here can also be found in a recent paper on entangled quantum states [12].

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