Entanglement measures and the quantum-to-classical mapping

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Abstract. A quantum model can be mapped to a classical model in one higher dimension. Here we introduce a finite-temperature correlation measure based on a reduced density matrix $\bar{\rho}_A$ obtained by cutting the classical system along the imaginary time (inverse temperature) axis. We show that the von Neumann entropy $\bar{S}_{\text{ent}}$ of $\bar{\rho}_A$ shares many properties with the mutual information, yet is based on a simpler geometry and is thus easier to calculate. For one-dimensional quantum systems in the thermodynamic limit we prove that $\bar{S}_{\text{ent}}$ is non-extensive for all temperatures $T$. For the integrable transverse Ising and XXZ models we demonstrate that the entanglement spectra of $\bar{\rho}_A$ in the limit $T \to 0$ are described by free-fermion Hamiltonians and reduce to those of the regular reduced density matrix $\rho_A$—obtained by a spatial instead of an imaginary time cut—up to degeneracies.

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

Entanglement is usually thought of as a quantum mechanical entity yet it is well known that the properties of quantum models can be computed from a classical model in one dimension higher [1]–[3]. Such an approach is particularly useful if one is interested in how entanglement builds up in a thermal state while lowering the temperature or during unitary time evolution.

Entanglement measures are maps from the space of density matrices (DMs) into the positive real numbers, which should adhere to a set of axioms [4, 5]. For bipartite pure states the von Neumann entropy of entanglement fulfils these criteria and provides a bridge into statistical mechanics and condensed matter physics. In particular, the reduced DM, whose eigenvalues determine the entanglement entropy, is at the heart of the density matrix renormalization group (DMRG) [6]. This numerical method gives a recipe for how to optimally approximate pure states of many-body systems by matrix product states [7] and is most successful in one dimension.

In experiments we are, however, usually dealing with mixed states about whose entanglement properties much less is known. Entanglement measures commonly used for pure states of multi-particle systems such as the entanglement entropy fail because they become extensive and thus no longer fulfil a boundary law. Furthermore, they cannot distinguish between classical and quantum correlations [4]. Entanglement measures which do distinguish between these different types of correlation involve extremizations over all possible decompositions of the DM and explicit results have only been obtained for small matrix dimensions [8]–[10]. Putting these fundamental difficulties aside, it is still useful to define correlation measures for thermal ensembles which go beyond the one- and two-point correlation functions traditionally studied in statistical mechanics and condensed matter physics.
matter physics. They might help to reveal, in particular, phase transitions with complex or topological order parameters.

In this paper we want to investigate how correlations, generated during imaginary time evolution, can be quantified. After a quantum-to-classical mapping we introduce as a new measure the von Neumann entropy of a reduced DM obtained by a partial trace in the imaginary time direction. This measure also cannot distinguish between quantum and classical correlations, but we will show that it shares many properties with the mutual information, which has recently attracted considerable interest as a correlation witness for many-body systems [11]–[14], yet is easier to calculate. The quantity introduced in this paper is also a natural choice from the perspective of numerical matrix product state algorithms: while the reduced DM obtained by a spatial trace is at the heart of the DMRG at \( T = 0 \), the reduced DM considered here is used in transfer matrix DMRG algorithms to study the finite-temperature properties of one-dimensional systems in the thermodynamic limit [15]–[19]. Although not further pursued here, the ideas discussed are also relevant for the entanglement generation during the real time evolution of a quantum system. The results obtained in the following can be generalized to this case by considering an analytical continuation which replaces the thermal DM by the time evolution operator.

2. Entanglement entropy and mutual information

The entanglement entropy for a bipartite system, \( S = A \cup B \), is defined as

\[
S_{\text{ent}}(A) = -\text{Tr} \rho_A \ln \rho_A
\]

where \( \rho_A = \text{Tr}_B \rho \), \( \text{Tr}_B \rho_A = 1 \), is a reduced DM obtained from the DM \( \rho \) of the system \( S \) by spatially tracing out part \( B \). If the system is in a pure state, then it is easy to show by a Schmidt decomposition that \( S_{\text{ent}} \equiv S_{\text{ent}}(A) = S_{\text{ent}}(B) \). This seems to point to a non-extensive scaling of \( S_{\text{ent}} \) with the surface between regions \( A \) and \( B \) [20]. Often, this is indeed the case and this behavior is called the entropic boundary law. However, violations of the boundary law are also known. Most importantly, the entanglement entropy scales logarithmically with the length of the considered region for critical one-dimensional systems [21, 22], instead of being constant as might be expected by the simple argument given above. Even more severe violations of the boundary law have been shown to exist in models with inhomogeneous interactions [23].

Here we want to study the mixed state described by the canonical DM \( \rho_c = \exp(-\beta H)/Z \), where \( \beta \) is the inverse temperature, \( H \) the Hamiltonian, and \( Z = \text{Tr} \rho_c \) the partition function. Calculating the entanglement entropy (1) for \( \rho = \rho_c \), one finds that \( S_{\text{ent}}(A) \neq S_{\text{ent}}(B) \) in general and that \( S_{\text{ent}} \) becomes extensive approaching the regular thermal von Neumann entropy for \( \beta \to 0 \) [22, 24]. This can be easily understood as follows. If all correlation lengths are much smaller than the extent of the considered subsystem \( A \), then the rest of the system \( B \) just acts as an additional bath. A way to partly correct this is to consider the mutual information given by

\[
I_{A,B} = S_{\text{ent}}(A) + S_{\text{ent}}(B) - S_{\text{th}}(S)
\]

where \( S_{\text{th}}(S) = -\text{Tr} \rho_c \ln \rho_c \) is the thermal von Neumann entropy. The thermal contribution is then explicitly subtracted ensuring that \( I_{A,B}(\beta \to 0) \to 0 \) as required. However, the mutual information is still not a proper entanglement measure because classical as well as
quantum correlations contribute. Furthermore, the evaluation of the mutual information is difficult because $S_{\text{ent}}$ is often inaccessible at finite temperatures. Instead, the Renyi entropy

$$ S_n(A) = \ln[\text{Tr}(\rho^n_A)]/(1 - n) \quad (3) $$

with $n$ integer is often used in equation (2) instead of the von Neumann entropy. However, even then the calculation is quite involved due to the complicated geometry required to obtain $\text{Tr}[\rho^n(A)]$ from generalized partition functions [22, 25, 11, 12, 14]. An obvious question is if related finite-temperature correlation measures can be defined which are easier to use in analytical and numerical calculations.

3. Coupled qubits

To explain and motivate the idea of a correlation measure based on a quantum-to-classical mapping, we start with two coupled qubits with Hamiltonian

$$ H = S_1 \cdot S_2 \quad (4) $$

where $S$ is a spin-1/2 operator. Any type of correlation or entanglement measure can, of course, easily be obtained in this case, because the Hamiltonian is just a $4 \times 4$ matrix. We believe, however, that this simple system is very helpful to shed some light on the following points. (a) Why and in which way does $S_{\text{ent}}$ fail as a correlation measure at finite temperatures? (b) What are possible mappings onto a one-dimensional classical model and how do we define new operators acting in an auxiliary space along the imaginary time axis?

Concerning point (a), let us consider first the imaginary time evolution starting from the separable state $|\uparrow\downarrow\rangle = (|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)/2 + (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)/2$. Time evolving with $e^{-\beta H}$ this state becomes

$$ |\Psi_\beta\rangle = \frac{\exp(-\beta/4)}{2}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) + \frac{\exp(3\beta/4)}{2}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) \quad (5) $$

and gets projected onto the maximally entangled singlet ground state for $\beta \to \infty$. A picture showing how the entangled state is formed out of the separable state can be obtained by the quantum-to-classical mapping. We discretize time into steps $\delta \beta$, writing $\rho_c = \tau^M/Z$, where $\tau = \exp(-\delta \beta H)$ and $M\delta \beta = \beta$. Rewriting the Hamiltonian as $H = \frac{1}{2} P_{1,2} - \frac{1}{4} \text{Id}_{1,2}$ we find

$$ \tau \approx \left(1 + \frac{\delta \beta}{4}\right) \text{Id}_{1,2} - \frac{\delta \beta}{2} P_{1,2} \quad (6) $$

where $\text{Id}_{1,2}$ is the identity and $P_{1,2}$ the operator permuting the spins at sites 1, 2 during the time step $\delta \beta$. A pictorial representation of the imaginary time evolution operator $\tau$ is shown in figure 1(a). Entanglement is thus being generated during imaginary time evolution by the braiding of the worldlines of the two spins. This is shown for one possible configuration of $\tau$-matrices in figure 1(b).

For the separable initial state $|\uparrow\downarrow\rangle$, the correlations created during imaginary time evolution can still be measured by $S_{\text{ent}}$, equation (1), using the pure state DM $\rho = |\Psi_\beta\rangle \langle \Psi_\beta|/\langle \Psi_\beta|\Psi_\beta\rangle$ and tracing out one of the spins (see figure 1(e)). When using the mixed state DM $\rho = \rho_c$, on the other hand, one finds $S_{\text{ent}} = \ln 2$ independent of temperature.
$S_{\text{ent}}$ fails as a correlation measure and the whole temperature dependence of the mutual information (see figure 1) stems from the thermal von Neumann entropy. The mutual information can thus easily be calculated and we find, in particular, $I_{A,B} \sim 3/32T^2$ for $T \to \infty$. Because both classical and quantum correlations are contributing, there is no 'sudden death' with temperature, i.e. an exponential decay, as might be expected for a true finite-temperature entanglement measure. Let us stress that $S_{\text{ent}}$ nevertheless remains a useful correlation measure as long as we are dealing with pure state DMs.

In the following, we want to use this insight to pursue a different perspective on the classical representation of the qubits shown in figure 1(b) by defining a transfer matrix operator, a method often used in statistical mechanics. One way to achieve this is to perform an alternating $45^\circ$ clockwise and anti-clockwise rotation of the $\tau$-plaquettes. This leads to the completely equivalent graphical representation shown in figure 1(c) with plaquettes $\tau_{R,L} = T_{R,L}\tau$, where $T_{R,L}$ is the right/left shift operator, respectively. Tracing over one pair of open indices, either 1, 1' or 2, 2', gives the reduced DM $\rho_A$, while tracing over both pairs gives the partition function $Z$. By moving the right $\delta$ bonds (lines in figure 1(c)) to the left and tracing over 1, 1' and 2, 2' we obtain the DM $\bar{\rho}$ acting in an auxiliary space along the imaginary time axis, which is discretized in steps of $\delta\beta$. $\bar{\rho}$, shown in figure 1(d), then consists of two columns, with the left column containing only right and left shift operators, $T_{R,L}$. We now investigate the reduced DM $\bar{\rho}_A = \text{Tr}_B\bar{\rho}$ obtained by taking a partial trace in auxiliary space, i.e. by tracing over the pairs of indices 3, 3' and 4, 4' as a function of temperature.
Figure 2. (a) Two-dimensional lattice obtained after the quantum-to-classical mapping. The shaded part is the QTM $T$. Performing the trace over regions $\bar{A}$ and $\bar{B}$ and the partial spatial trace over $B$ yields $\bar{\rho}_A$, while tracing over $A$ and $B$ and taking the partial trace over $\bar{B}$ yields $\bar{\rho}_\bar{A}$. In both cases one obtains a torus with a cut. (b) Geometry to calculate $\text{Tr}\bar{\rho}_A^2$. Part $\bar{B}$ consists of two small cylinders (green dots mean that upper and lower free indices should be traced over) while part $A$ is one large cylinder.

4, 4'. Note that regions $\bar{A}, \bar{B}$ always have to contain an even number of $\tau_{RL}$-plaquettes so that the numbers of right and left shift operators are the same. A discretization using more than four plaquettes would, in the simple case considered, just add additional zero eigenvalues to $\bar{\rho}_\bar{A}$. The entanglement measure $\bar{S}_{\text{ent}}(\bar{A}) = -\text{Tr}\bar{\rho}_\bar{A}\ln\bar{\rho}_\bar{A} = \bar{S}_{\text{ent}}(\bar{B})$ is thus well defined and can easily be calculated (see figure 1(e)) with $\lim_{T \to 0}\bar{S}_{\text{ent}} = 2\ln 2$ and $\bar{S}_{\text{ent}} \sim 3(1+6\ln 2 + 2\ln T)/64T^2$ for $T \to \infty$. Up to a logarithmic term, $\bar{S}_{\text{ent}}$ thus shows the same $1/T^2$-decay at high temperatures as $\mathcal{I}_{A,B}$. To summarize, we can obtain a correlation measure which is useful even for a mixed state by first performing a quantum-to-classical mapping and second taking a partial trace in the auxiliary space along the imaginary time direction instead of the commonly used partial trace in space.

4. One-dimensional models

Next, we want to generalize these considerations to one-dimensional quantum systems. A Hamiltonian with short-range interactions can always be written as $H = \sum_j h_{j,j+1}$, possibly in an enlarged unit cell. By using a Trotter–Suzuki decomposition, the system can be mapped onto a two-dimensional classical system in much the same way as we have mapped the qubits onto a one-dimensional classical system. A pictorial representation is shown in figure 2(a), where each plaquette is given by $\tau_{RL} = T_{RL}\exp(-\delta\beta h_{j,j+1})$. Note that $[h_{j,j+1}, h_{k,k+1}] \neq 0$ in general, so the mapping induces an error which is of the order of $(\delta\beta)^2$ for the partition function.

The canonical DM $\rho_c$ for periodic boundary conditions is shown in figure 2(a) with the l.h.s. and r.h.s. indices at the same imaginary time step traced over. Tracing instead over the upper and lower indices and leaving the indices on the l.h.s. and r.h.s. open, we obtain the DM $\bar{\rho} = T^L/Z$ where $T$ is a quantum transfer matrix (QTM) acting in auxiliary space. The partition function is given by $Z = \text{Tr}_{A,B}\rho_c = \text{Tr}_{\bar{A},\bar{B}}\bar{\rho}$. For $T > 0$
the thermodynamic limit can now be performed exactly with \( \lim_{L \to \infty} \bar{\rho} = |\Psi_R\rangle \langle \Psi_L| \). Here \( |\Psi_R\rangle \) and \( \langle \Psi_L| \) are the left and right eigenvectors belonging to the largest eigenvalue of \( T \) with \( \langle \Psi_L| \Psi_R\rangle = 1 \). This property can be easily understood physically because all correlation lengths—determined by the logarithm of the ratio of the leading to subleading eigenvalues of \( T \) [26]—have to stay finite. Thus the contributions of other eigenstates have zero weight in the thermodynamic limit and \( \bar{\rho} \) becomes a projector onto the ground state in auxiliary space. Another important point to note is that, in general, quantum lattice models do have correlations incommensurate with the lattice. In the transfer matrix formalism such incommensurabilities manifest themselves through complex eigenvalues. Therefore \( T \) cannot be a symmetric matrix.

The reduced DM \( \bar{\rho}_A = \text{Tr}_B \bar{\rho} \) is obtained by tracing over the indices in region \( B \). \( \bar{\rho}_A \) is also non-symmetric, so the spectrum does not have to be real. In numerical transfer matrix DMRG calculations for various bosonic, fermionic and spin models a real spectrum is found up to very small imaginary parts which sporadically seem to occur due to numerical instabilities of the diagonalization routine. A general proof has so far, however, not been given. In the following we confirm that the eigenvalues of \( \bar{\rho}_A \) are real for the transverse Ising and the XXZ model by relating both spectra to those of a two-dimensional Ising model. Crucially, it is in any case easy to show using a Schmidt decomposition and choosing biorthonormal sets of right and left basis vectors that \( \bar{S}_{\text{ent}}(A) = \bar{S}_{\text{ent}}(B) \). \( \bar{\rho} = |\Psi_R\rangle \langle \Psi_L| \) being a projector thus guarantees that \( \bar{S}_{\text{ent}} \) is non-extensive for all temperatures \( T \). It is thus quite natural to replace the projector \( \rho \) onto the ground state, considered for zero temperature, with the projector in auxiliary space, \( \bar{\rho} \), for an infinite one-dimensional system at finite temperatures. \( \rho \), on the other hand, is not a projector for \( T > 0 \) and \( S_{\text{ent}}(T) \) is very difficult to calculate. Instead, the mutual information (2) based on the Renyi entropy (3) with \( n = 2 \) is often used. A quantum-to-classical mapping then yields the geometry for \( \text{Tr}(\rho_A^2) \) shown in figure 2(b). One can now again try to perform the thermodynamic limit by defining separate QTMs for part \( A \) and part \( B \) of the system. Each one of them projects onto its ground state in auxiliary space; however, an evaluation of \( S_2(A) \) requires us to calculate the overlap between the two different ground states [14] and is thus much harder than obtaining \( \bar{S}_{\text{ent}} \), where no such overlap has to be calculated. In the following, we study the scaling properties of \( \bar{S}_{\text{ent}}(T) \) and the spectra of \( \bar{\rho}_A \) for a symmetric cut \( \bar{A} = \bar{B} = \beta/2 \) using analytical calculations as well as a numerical transfer matrix renormalization group (TMRG) algorithm [15]–[19].

4.1. Transverse Ising model

We start with the transverse Ising model

\[
H = \sum_j \left( \sigma_j^x \sigma_{j+1}^x + \lambda \sigma_j^y \right)
\]  

(7)

where \( \sigma \) are the Pauli matrices. This model shows a second order phase transition at \( \lambda = 1 \) [3]. The eigenvalues \( \xi_i \) of \( \bar{\rho}_A \) in the low-temperature limit are shown exemplarily in figures 3(a) and (c) and are equally spaced. The degeneracies of the eigenvalues, starting with the largest ones, are given by 2, 4, 6, 12, . . . for \( \lambda < 1 \) and 1, 2, 1, 2, 4, 4, 5, 6, . . . for \( \lambda > 1 \). This simple structure can be understood analytically completely analogously to the spectrum of the regular reduced DM \( \rho_A \) at \( T = 0 \) obtained by a spatial cut, which has been investigated by Peschel et al [27]. In both cases the reduced DM can be regarded as
Figure 3. TMRG results are denoted by symbols. Main: $S_{\text{ent}}$ for various $T$ and exact result for $T = 0$ (solid line). Eigenvalues $\xi_i$ of $\bar{\rho}_A$ for (a) $\lambda = 0.8$ and (c) $\lambda = 1.2$ at $T = 0.02$. The free-fermion levels from the analytical solution are denoted by dashed lines. (b) $S_{\text{ent}}(T)$ for $\lambda = 1$ and low-temperature fit $S_{\text{ent}} = -0.167 \ln T + 0.402$.

the partition function of a strip of the two-dimensional classical Ising model [27]–[29]. The only difference is due to the periodic boundary conditions in the imaginary time direction. Region $\bar{A}$ therefore has two boundaries instead of only one as for the regular reduced DM in a system with open boundaries considered in [27]. The spectrum can then be calculating by using corner transfer matrices (CTMs) for the two-dimensional Ising model. We can write $\bar{\rho}_A = e^{-H_{\text{CTM}}/T}/\text{Tr} e^{-H_{\text{CTM}}}$, where $H_{\text{CTM}} = \sum \epsilon_j n_j$ is a free-fermion Hamilton operator. For $\lambda > 1$ all single particle levels are twofold degenerate, $n_j = 0, 1, 2$, and given by

$$\epsilon_j = (2j + 1)\pi K(\sqrt{1 - 1/\lambda^2})/K(1/\lambda)$$

where $K(x)$ is the complete elliptic integral of the first kind. For $\lambda < 1$ we have

$$\epsilon_j = j\pi K(\sqrt{1 - \lambda^2})/K(\lambda)$$

where $\epsilon_0$ is non-degenerate and all other levels twofold degenerate [30]. In both cases the energy levels are exactly the same as described in [27]. The twofold degeneracy is the consequence of the periodic boundary conditions in the imaginary time direction. Only the energy level $\epsilon_0$ for $\lambda < 1$ plays a special role and stays non-degenerate. Using the known results for the spectrum of $\rho_A$, Calabrese and Cardy have calculated $S_{\text{ent}}$ for the Ising model [22]. From the analytical results for the spectrum of $\bar{\rho}_A$ in the zero temperature limit given above we can similarly calculate $S_{\text{ent}}(T \to 0)$. The result is shown as a solid line in figure 3 and is in excellent agreement with the TMRG data. Calabrese and Cardy have shown, furthermore, that right at the critical point the regular entanglement entropy $S_{\text{ent}}$ for an interval of length $\ell$ in an infinite chain shows a logarithmic divergence with system size, $S_{\text{ent}} = (c/3) \ln \ell + C_1$, with central charge $c = 1/2$ and a non-universal constant.
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Figure 4. (a) One-parameter fits (lines) of TMRG data (symbols) for $T/J \leq 0.1$ according to equation (10) with $c = 1$, $v$ as known from the Bethe ansatz, and $C_1$ as indicated. (b) Spectrum of $\bar{\rho}_A$ for $\Delta = 10$ and $T/J = 0.02$. The numbers give the multiplicities of each level (total in brackets); the dashed lines mark the free-fermion levels.

$C_1$ [22]. From this result it follows immediately by a conformal mapping that

$$\bar{S}_{\text{ent}}(T) = \frac{c}{3} \ln(v/T) + C_1$$

with $v$ being the velocity of the elementary excitations. This result is universal for critical systems. For the transverse Ising model it is in excellent agreement with a two-parameter fit of the numerical data, which yields $v = 1$ and $C_1 \approx 0.402$; see figure 3(b).

4.2. XXZ model and boundary locality

As a further example, we calculate the spectrum of $\bar{\rho}_A$ and $\bar{S}_{\text{ent}}$ for the XXZ model,

$$H = J \sum_j \{ S_j^x S_{j+1}^x + S_j^y S_{j+1}^y + \Delta S_j^z S_{j+1}^z \} .$$

Here $S$ is a spin-1/2 operator and $\Delta$ parametrizes the exchange anisotropy. The model is critical for $-1 < \Delta \leq 1$ with central charge $c = 1$. As shown in figure 4(a) for three different values of $\Delta$, equation (10) does indeed describe $\bar{S}_{\text{ent}}$ for $T \ll J$. As for the transverse Ising model, the spectrum of the regular reduced DM $\rho_A$ in the non-critical case $\Delta > 1$ can be constructed by mapping to a two-dimensional Ising model [27]. We find again that the same mapping can also be applied to find the spectrum of $\bar{\rho}_A$ at low temperatures; see figure 4(b). The total degeneracies of the free-fermion levels are the same as for the transverse Ising model with $\lambda < 1$; however, now [27]

$$\epsilon_j = 2j \cosh^{-1}\Delta .$$

In the case of the regular reduced DM $\rho_A$ the degenerate levels can be further classified by their spin, $S_{\text{tot}}^z = \sum_j S_j^z$, which commutes with the Hamiltonian and is thus a good
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quantum number. For the QTM $\mathcal{T}$ one can define a good quantum number as $\bar{S}_{R,L} = \sum_k (\pm 1)^k (S_k^z)_{R,L}$. Here $(S_k^z)_{R,L}$ acts at site $k$ in the discretized imaginary time direction on the r.h.s. ($R$), respectively l.h.s. ($L$), of the transfer matrix $\mathcal{T}$. Matrix elements of $\mathcal{T}$ can thus only be non-zero if $\bar{S}^z \equiv \bar{S}_R^z = \bar{S}_L^z$ and eigenvalues of $\bar{\rho}_A$ can be classified according to $\bar{S}^z$; see figure 4(b).

For $\rho_A$ it has been shown that the spectrum as a function of $S_{\text{tot}}^z$ can be constructed for $\Delta \gg 1$ by local perturbation theory in the spin exchange operator [31]. A similar local perturbation theory also works for the QTM $\mathcal{T}$ and the degeneracies of each level for $\bar{\rho}_A$ as a function of $\bar{S}^z$ are exactly the same as for $\rho_A$ classified by $S_{\text{tot}}^z$ for a system with periodic boundary conditions. This demonstrates explicitly that a boundary law also holds for $\bar{\rho}_A$.

5. Two-dimensional models

The quantum-to-classical mapping of a finite two-dimensional system of extent $L_1 \times L_2$ leads to a three-dimensional system with dimensions $\beta \times L_1 \times L_2$. In order to calculate the mutual information $I_{A,B}$, equation (2), following a spatial cut one can use the replica trick [22]. However, from numerical data it is very difficult to obtain the entanglement entropy $S_\text{ent} = \lim_{n \to \infty} S_n$. Instead, the mutual information based on the Renyi entropy $S_2$ has been obtained from the three-dimensional generalization of the geometry shown in figure 2(b) by quantum Monte Carlo (QMC) simulations [25, 11, 12]. However, the non-trivial geometry with periodicity $\beta$ in region $A$ and $\beta/2$ in region $B$ makes the calculations more difficult than a standard QMC calculation. The numerical calculation of $S_\text{ent}$, in contrast, is also straightforward in two dimensions because the geometry is the same as in a standard QMC calculation. For $L_1$ and $L_2$ both finite, one can use the mutual information $I_{A,B} \equiv S_\text{ent}(A) + S_\text{ent}(B) + \text{Tr} \ln \bar{\rho}$ to detect finite-temperature phase transitions. Furthermore, one can take the thermodynamic limit in one of the spatial dimensions so that $\rho$ becomes again a projector, implying $\lim_{T \to \infty} S_\text{ent} = 0$, so that subtraction of a ‘thermal part’ is not required.

6. Discussion

We have analyzed finite-temperature correlation measures for quantum systems from the perspective of a quantum-to-classical mapping. In particular, we have studied the von Neumann entropy of a reduced DM obtained by cutting the classical system along the imaginary time axis at $\beta/2$ and tracing out the degrees of freedom in one half of the system. We have motivated this correlation measure by studying two coupled qubits and shown that its value depends on the braiding of the worldlines of the spins during imaginary time evolution. Furthermore, we have demonstrated that this measure has the same zero temperature limit and the same high-temperature asymptotics (up to a logarithmic correction) as the mutual information.

For one-dimensional quantum systems it is well known that the quantum-to-classical mapping makes it possible to take the thermodynamic limit by defining a transfer matrix $\mathcal{T}$ which evolves along the spatial direction. All thermodynamic quantities are then determined by the largest eigenvalue of this transfer matrix and one can define a DM $\bar{\rho} = |\Psi_R\rangle \langle \Psi_L|$, where $|\Psi_R\rangle$ $(|\Psi_L\rangle)$ are the right (left) eigenvectors of $\mathcal{T}$ belonging to the largest eigenvalue. Studying the entanglement properties of this projector onto the ground
state in auxiliary space by performing a partial trace along the imaginary time axis is a natural generalization of studying the entanglement properties of the projector onto the physical ground state, \( \rho = |\Psi_0\rangle\langle\Psi_0| \), at zero temperature. In particular, the DM being a projector guarantees that the corresponding von Neumann entropy \( \bar{S}_{\text{ent}} \) of the reduced DM \( \bar{\rho}_A \) will fulfill a boundary law.

To understand the properties of the reduced DM \( \bar{\rho}_A \) better, we have studied two examples, the Ising and the XXZ chain, in detail. In both cases the spectrum of \( \bar{\rho}_A \) can be calculated analytically in the zero temperature limit by a mapping to the two-dimensional Ising model, and the results are identical (up to degeneracies) to the ones obtained for the standard reduced DM at zero temperature [27]. Our results show that transfer matrix DMRG algorithms—which use \( \bar{\rho}_A \) to choose the states kept in a truncated Hilbert space and have been extensively used for many years—are as efficient in simulating one-dimensional quantum systems in the thermodynamic limit at finite temperatures as regular DMRG algorithms are for finite systems at \( T = 0 \). For critical systems we find by a conformal mapping that \( \bar{S}_{\text{ent}} \) shows logarithmic scaling with temperature, with the prefactor being determined by the central charge.

Finally, we have suggested that \( \bar{S}_{\text{ent}} \) can be used for two- and three-dimensional quantum systems to investigate finite-temperature phase transitions. For quantum Monte Carlo calculations, in particular, this might be a viable and—due to the simpler geometry—easier approach than calculating Renyi entropies.

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