Criticality, the Area Law, and the Computational Power of Projected Entangled Pair States

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(Received 27 January 2006; published 6 June 2006)

The projected entangled pair state (PEPS) representation of quantum states on two-dimensional lattices induces an entanglement based hierarchy in state space. We show that the lowest levels of this hierarchy exhibit a very rich structure including states with critical and topological properties. We prove, in particular, that coherent versions of thermal states of any local $2D$ classical spin model correspond to such PEPS, which are in turn ground states of local $2D$ quantum Hamiltonians. This correspondence maps thermal onto quantum fluctuations, and it allows us to analytically construct critical quantum models exhibiting a strict area law scaling of the entanglement entropy in the face of power law decaying correlations. Moreover, it enables us to show that there exist PEPS which can serve as computational resources for the solution of NP-hard problems.

DOI: 10.1103/PhysRevLett.96.220601 PACS numbers: 05.50.+q, 03.67.Mn, 05.70.Jk, 89.70.+c

The concept of entanglement plays a central role in both fields of quantum information theory and of strongly correlated systems. In quantum information theory it lies at the heart of many applications and it is viewed as a resource for various information processing tasks. In condensed matter theory, entanglement is one of the roots for the notorious complexity of quantum many-body systems: its presence necessitates a description within an exponentially growing Hilbert space and it is intimately connected with many of the fascinating properties which quantum matter can exhibit at small temperatures.

Many fundamental questions arise at the crossing of these fields: how is entanglement related to the power of quantum computation on the one hand, and the difficulties of classical simulations on the other? What is the scaling of the entanglement entropy in spin systems, its relation to criticality, and the appearance of topological quantum order? All these questions can be addressed very easily within the framework of so-called projected entangled pair states (PEPS)—this is the intention of this Letter. We will see, in particular, that all the above-mentioned properties emerge naturally already within the simplest classes of PEPS which include cluster, toric code, and resonating valence bond states. This will enable us to settle a recent debate about the relation between criticality and entropy scaling, and it allows us to find computational resources for the solution of NP-hard problems. The central tool of the Letter is a general correspondence between thermal states of classical $2D$ spin models and $2D$ quantum states with a simple PEPS representation. This correspondence substitutes thermal by quantum fluctuations while preserving the correlations, and it thus allows to map temperature driven classical phase transitions to zero-temperature quantum phase transitions.

We begin by recalling the PEPS formalism, which was introduced in the context of numerical renormalization group methods for simulating strongly correlated quantum spin systems [1,2]. PEPS can be viewed as generalizations of the Affleck, Kennedy, Lieb, and Tasaki (AKLT) valence bond solids [3] to arbitrary lattices and dimensions. Consider an arbitrary connected graph where each of N vertices corresponds to a quantum system, a *spin*, with d degrees of freedom. A PEPS $|\Psi\rangle \in \mathbb{C}^{d^N}$ is then constructed by (i) assigning to each vertex as many virtual spins of dimension D as there are adjacent edges, (ii) putting a maximally entangled state $|I\rangle = \sum_{i=1}^{D} |ii\rangle$ onto each edge, and (iii) mapping the virtual onto the physical spins by applying a linear map $P{:}\mathbb{C}^D \otimes \cdots \otimes \mathbb{C}^D \to \mathbb{C}^d$ at each vertex. Naturally, the graph is chosen according to the physical symmetry, and although most of the following holds in general we will consider square lattices throughout. Different choices of P lead to different quantum states, and in the case of a square lattice all these PEPS live on a NdD^4 dimensional manifold.

The power of the PEPS formalism is based on two points. First, every state has a PEPS representation [4] as long as D can become very large. Hence, with increasing D this representation induces a hierarchy in the space of states, from product or mean-field states ($D = 1$) to more and more entangled ones; the manifold of D-dimensional PEPS is indeed embedded in the one with $D' > D$. Second, it appears that many states arising in physics are very well approximated by the lower levels of this hierarchy [5]. This makes them a powerful variational class for numerical renormalization group methods on the one hand [1,4], and an interesting test bed for all kinds of quantum many-body questions on the other [6].

Quantum-classical correspondence.—Consider a classical two-body spin Hamiltonian of the form $H(\sigma_1, \ldots, \sigma_N) = \sum_{(i,j)} h(\sigma_i, \sigma_j)$ with $\sigma_i = 1, \ldots, d$ and respective partition function $Z = \sum_\sigma \exp[-\beta H(\sigma)]$ at inverse temperature β. From this, a corresponding quantum state can be constructed by using the Boltzmann weights as superposition

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coefficients such that

$$|\psi_{H,\beta}\rangle = \frac{1}{\sqrt{Z}} \sum_{\sigma_1,\ldots,\sigma_N} e^{-(\beta/2)H(\sigma_1,\ldots,\sigma_N)} |\sigma_1, \ldots, \sigma_N\rangle. \quad (1)$$

We will see that $|\psi_{H,\beta}\rangle$ has the following properties: (i) for diagonal observables it gives rise to the same expectation values and correlations as the classical thermal state, (ii) it has a simple PEPS representation with $D = d$, (iii) it is the ground state of a local quantum Hamiltonian, and (iv) when considering asymptotically large systems ($N \to \infty$) the scaling of the entropy of a block of spins obeys a strict area law. Whereas (i) is a direct consequence of the construction, (iii) and (iv) are implied by the PEPS parametrization. In order to see the latter we rewrite the state as

$$|\psi_{H,\beta}\rangle = \frac{1}{\sqrt{Z}} \exp\left[-\frac{\beta}{2}\sum_{(i,j)} \hat{h}_{ij}\right] |+, \cdots, +\rangle, \quad (2)$$

where $|+\rangle = \sum_{s=1}^{d} |s\rangle$ and $\hat{h}_{ij}$ is a diagonal operator acting on sites i, j as $\hat{h}_{ij}|\sigma_i, \sigma_j\rangle = h(\sigma_i, \sigma_j)|\sigma_i, \sigma_j\rangle$. Following Eq. (2) we can think of the state $|\psi_{H,\beta}\rangle$ as being constructed from the product state $|+, \cdots, +\rangle$ by applying (nonunitary) gates $\exp[-\beta\hat{h}/2]$ to all neighboring spins. In fact, we may interpret Eq. (2) as a quantum cellular automaton evolution in imaginary time. As explained in [2], a nonlocal gate like $\exp[-\beta\hat{h}/2]$ can be reexpressed by local operations which act additionally on an auxiliary maximally entangled state. More specifically, we take operators $\mathcal{P}, \mathcal{P}'$:$\mathbb{C}^{d^2} \to \mathbb{C}^d$, each acting as $\mathcal{P}|s, k\rangle = |s\rangle\langle\varphi_s|k\rangle$. Then we obtain indeed $\exp[-\beta/2\hat{h}] = (\mathcal{P} \otimes \mathcal{P}')|I\rangle$ if we choose the vectors $\varphi_s, \varphi'_{s'}$ such that $\sum_{k=1}^{d}\langle\varphi_s|k\rangle\langle\varphi'_{s'}|k\rangle = \exp[-\beta/2h(s, s')]$ which is always possible, e.g., by a singular value decomposition. Applying these gates to all edges leads then to the desired PEPS representation.

As an example, consider the Ising model on a $2D$ square lattice with $H(\sigma) = -\sum_{(i,j)}\sigma_i\sigma_j$, $\sigma_i = \pm 1$. In this case we can choose $\varphi_s = \varphi'_s$ such that $\langle\varphi_s|k\rangle$ are the matrix elements of the square root of the matrix h. Applying all the gates gives then rise to a PEPS [7] with

$$P = |0\rangle\langle\varphi_0|\langle\varphi_0|\langle\varphi_0|\langle\varphi_0| + |1\rangle\langle\varphi_1|\langle\varphi_1|\langle\varphi_1|\langle\varphi_1|.$$

Clearly, the expectation values of Pauli S_z operators in $|\psi_{H,\beta}\rangle$ equal the classical expectation values. In the quantum case, however, we do not only have diagonal observables, but also nondiagonal ones like S_x. Surprisingly, their expectation values are determined by classical ones as well, like

$$\langle\psi_\beta|S_x^1|\psi_\beta\rangle = \sum_{\sigma_1,\sigma_2,\ldots} e^{-\beta H(\sigma_1,\sigma_2,\ldots)} e^{\beta\sum_{(1,j)}\sigma_1\sigma_j},$$

where the last term is a local 5-body expectation value in the classical Gibbs state. In general, every local expectation value in the quantum state corresponds to a local expectation value in the classical state, where the region the observable acts on is enlarged at most by the interacting neighborhood.

Before continuing, it should be noted that several results related to the above classical-quantum correspondence can be found in the literature: a connection between so-called Rokshar-Kivelson points and classical stochastic models was recently made in [8] and between Hamiltonians and rapidly mixing reversible Markov chains in [9]. In [10] a generalization of the AKLT state on $2D$ lattices was considered and demonstrated that it can be mapped onto a classical vertex model. The PEPS formalism, discussed in the present Letter, provides a very natural framework for describing and generalizing those results.

Criticality and the area law.—Recently a lot of attention has been devoted to the scaling of the entanglement entropy [6,11–13]. That is, given a ground state, how does the entropy of a contiguous subsystem scale with the size of the latter? Originally appearing in the context of black holes, the renewed interest in this question comes from the investigation of quantum phase transitions and the quest for powerful ansatz states for the classical simulation of quantum systems. The entropy of a block of spins quantifies the amount of entanglement of that block with the outside, and it could be expected to increase monotonously both as a function of the area of the boundary L_b and of the correlation length $\xi_{\rm corr}$.

In $1D$ it is known that critical states corresponding to a conformal field theory exhibit a logarithmic divergence of the entropy $S \sim \log L$ (L being the length of the subsystem), whereas there seems to be a saturation scaling to $\log\xi_{\rm corr}$ for all noncritical systems [11]. In $\mathcal{D} > 1$ dimensions, quasifree systems of bosons [12] and fermions [13] have been studied. Whereas in the noncritical (gapped) bosonic case there is a strict area law $S = O(L^{\mathcal{D}-1})$ (for a cube with edge length L), this is violated in the gapless case of fermions, where $S \sim L^{\mathcal{D}-1}\log L$. This naturally rises the question about a one-to-one correspondence between criticality and a violation of the area law in the form $S \sim L^{d-1}\log L$. Phrased differently, it raises the question whether the leading term in the entropy (which scales like the area) must have a prefactor that has, at criticality, a singular (and hence universal) dependence on a coupling constant (as is the case in $1D$); is the leading term in the entropy in the case of a critical system generated by nonuniversal short distance physics or by the long-range critical modes?

The PEPS formalism together with the above classical-quantum correspondence enables us now to answer this question in the negative in a very simple way: consider the classical $2D$-Ising system, which is known to become critical in the thermodynamic limit at $\beta_c = \frac{1}{2}\ln(1 + \sqrt{2})$. The corresponding quantum state $|\psi_{\beta_c}\rangle$ is the exact ground state of a local Hamiltonian (as shown in the next section) and will have exactly the same correlations $\langle S_z^0 S_z^r\rangle \sim 1/\sqrt{r}$, which now reflect critical quantum rather than thermal fluctuations. In spite of this, the state obeys a strict area

law bound $S \leq 4L$ due to the PEPS representation with $D = 2$ since the entropy is solely generated by breaking $4L$ entangled bonds at the boundary (see Fig. 1). It is an open question whether this behavior is generic or the consequence of the fact that the considered example has a dynamic critical exponent $z = 2$.

Parent Hamiltonians.—Every PEPS with finite D is (on a sufficiently large lattice) the ground state of a local Hamiltonian. The standard construction of such parent Hamiltonians identifies projectors onto null spaces of reduced density operators with the interaction terms in the Hamiltonian [3,6]. Here we will follow a different approach, related to the one described in [8,9], which is adapted to PEPS constructed from classical models and allows us to prove uniqueness and existence of a gap above the ground state energy for $\beta < \beta_c$.

Consider any ergodic local Markov process obeying detailed balance and converging to the equilibrium distribution of the classical model at inverse temperature β (e.g., by using Metropolis Monte Carlo or general Glauber dynamics). The stochastic transition matrix corresponding to the Markov process can be written as a sum $M(\beta) = \sum_k M_k(\beta)$ where each $M_k(\beta)$ acts locally and obeys detailed balance. The latter requires $p_a(\beta)[M_k(\beta)]_{a,b} = p_b(\beta)[M_k(\beta)]_{b,a}$ with $p_a(\beta) = \exp[-\beta H(a)]/Z$ and a, b denoting a particular configuration of the N spins. This is equivalent to imposing that all the matrices

$$P_k(\beta) = e^{-(\beta/2)\sum_{(ij)} \hat{h}_{ij}} M_k(\beta) e^{\beta/2 \sum_{(ij)} \hat{h}_{ij}}$$

are symmetric. Obviously, the operator $\sum_k P_k(\beta)$ is symmetric and has exactly the same eigenvalues as $\sum_k M_k(\beta)$ since they are connected by a similarity transformation. Furthermore, all $P_k(\beta)$ are local operators if the $M_k(\beta)$ were local. Note that $\mathbb{1} - \sum_k M_k(\beta)$ only has non-negative eigenvalues with the equilibrium distribution corresponding to eigenvalue 0. We thus define the Hamiltonian $H(\beta) = 1 - \sum_k P_k(\beta) \geq 0$ which is a sum of local operators such that by construction $|\psi_\beta\rangle$ is the ground state of $H(\beta)$. Moreover, $H(\beta)$ is gapped iff the stochastic matrix $M(\beta)$ has a gap. In this way the gap in the quantum Hamiltonian corresponds to the rate of convergence to equilibrium of the Markov process. In fact, the existence of a gap in $M(\beta)$ for $\beta < \beta_c$ was proven in [14] for a class of models including the $2D$ Ising model. At precisely the critical point, Monte Carlo methods exhibit a slowing down, leading to a gapless critical quantum Hamiltonian. In fact, power law decaying correlations imply that the Hamiltonian has to be gapless [15].

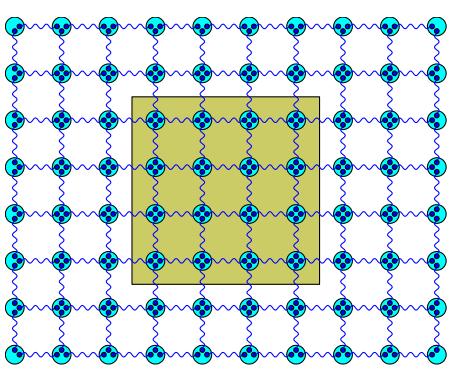

FIG. 1 (color online). The entropy of a block of spins in a PEPS scales like the perimeter of the block: the Schmidt rank of the reduced density operator of the considered block of spins is bounded above by the product of the Schmidt ranks of the broken bonds.

Computational power of PEPS.—In this section we will treat the PEPS as a resource for computational tasks. Given a source (black box) which can produce all D-dimensional PEPS, and given the ability of performing arbitrary local measurements, what kind of computational problems can be solved efficiently? This question is clearly inspired by the cluster state computational model [16]. In fact, it was shown in [2] that the cluster state is a PEPS with $D = 2$. Moreover, it is known to be a resource state for universal quantum computation, i.e., it enables us for instance to solve a typical NP problem—factorization—by merely performing local measurements. Since PEPS with $D = 1$ are product states, $D = 2$ is the simplest class in which useful resources can be expected. Exploiting the above formalism, one can show that there are other powerful resource states within this class, which even enable the efficient solution of NP-hard problems. In order to see this, note that given a quantum state $|\psi_\beta\rangle$ which corresponds to a classical Hamiltonian, we can efficiently determine expectation values in the classical Gibbs state by performing local (diagonal) measurements on $|\psi_\beta\rangle$. For $\beta \to \infty$ we can for instance *measure* the ground state energy [17]. This is, in particular, true for the $D = 2$ PEPS corresponding to a two-dimensional Ising spin glass within a magnetic field. This task was, however, shown to be an NP-hard problem [19]. Similarly, the determination of the partition function of the Potts model ($D > 2$) is known to be $\#P$ hard and tightly connected to hard problems in knot theory. As the task of calculating expectation values of PEPS can be done by contracting a network of tensors arranged on a square lattice [1], the above arguments prove that such a contraction of tensors is in general a NP-hard problem [20].

The approach of encoding the solution to an NP-hard problem into a quantum state is reminiscent of adiabatic quantum computing [18] which, however, deals typically with ground states of $1D$ albeit nonlocal Hamiltonians. In fact, one possible way of generating PEPS would be by adiabatic means with the usual caveat concerning the gap of the system. However, as in the case of the cluster state, there might be better ways of generating these states since after all we have an efficient *local* parametrization. The above observations make the following problem very interesting: what subclass of PEPS can be generated efficiently?

Let us finally show that two other classes of states, important for quantum information and condensed matter theory, are contained within small-D PEPS as well:

Toric code states introduced in the context of quantum error correction are very interesting as they exhibit nontrivial topological properties [21]. In the case of an infinite square lattice, the toric code is the ground state of a Hamiltonian consisting of local commuting projectors, each of them annihilating the ground state. The state can again be written in terms of the (zero-temperature) Boltzmann weights of a classical statistical model

$$|\psi_{\rm tor}\rangle \simeq \lim_{\beta\to\infty} \exp\left(+\frac{\beta}{2}\sum_{\square_i} S_z^{\alpha_i} S_z^{\beta_i} S_z^{\gamma_i} S_z^{\delta_i}\right)|++\cdots+\rangle,$$

where $\square_i$ denotes the ith plaquette in the lattice with the spins on the edges. We can again represent the commuting nonlocal gates by introducing entangled auxiliary degrees of freedom and applying local operations. We obtain projectors of the form

$$P_e = |0\rangle\langle\Psi^+|_{12}\langle\Psi^+|_{34} + |1\rangle\langle\Psi^-|_{12}\langle\Psi^-|_{34}$$
$$P_o = |0\rangle\langle\Psi^+|_{14}\langle\Psi^+|_{23} + |1\rangle\langle\Psi^-|_{14}\langle\Psi^-|_{23},$$

where $|\psi^\pm\rangle = |00\rangle \pm |11\rangle$ and P_e, P_o act on the even and odd sites of the bipartite lattice, respectively (the labels 1.4 denote the virtual qubits in clockwise order). Hence it is again a simple PEPS with $D = 2$ exhibiting nontrivial topological behavior. The PEPS formalism seems to provide a promising avenue for generating other states exhibiting those fascinating properties.

Resonating valence bond states (RVB) have been studied extensively in the context of strongly correlated systems [22]. These states exhibit topological quantum order and do not seem to have any classical statistical model associated to them because the wave function contains negative weights. For the case of simplicity, let us consider the simplest RVB state which is the equal weight superposition of all possible coverings of singlets over nearest neighbors on a square lattice. This RVB is equivalent to the PEPS defined by

$$P = |0\rangle(\langle 0222| + \langle 2022| + \langle 2202| + \langle 2220|) + |1\rangle$$
$$\times(\langle 1222| + \langle 2122| + \langle 2212| + \langle 2221|)$$

acting on virtual *singlets* of the form $|S\rangle = |01\rangle - |10\rangle + |22\rangle$ distributed between all nearest neighbors. Interestingly, we need $D = 3$ in this case, and again the area law is automatically proven (i.e., the entropy of a block of spins scales like the boundary). In a similar way, RVB with singlets distributed beyond nearest neighbors can be constructed.

In summary, we found that already the lowest levels of the PEPS hierarchy exhibit an enormously rich structure—they contain highly interesting states for quantum information (e.g., cluster and toric code states) as well as for condensed matter theory (e.g., critical and RVB states). This makes them an interesting variational class for numerical methods and a rich test bed for quantum many-body questions. Based on a classical-quantum correspondence we were able to find critical quantum models whose entropy scaling contrasts with the one for Fermions [and corresponding spin models [23]]. Moreover, it yielded a local description of simple PEPS encoding the solution of NP-hard problems.

Work supported by the Gordon and Betty Moore Foundation, European projects, der Bayerischen Staatsregierung and MEC MTM2005-00082.

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