Multiparty pure entangled states and local measurement with LHV models and efficient classical sampling via the PEPS formalism

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The difficulty of simulating quantum systems on classical computers has attracted considerable attention over many years. While the origin of this difficulty is still to be fully understood, the entanglement of quantum states and dynamics plays a role in many cases. In the context of many-body physics, overcoming this problem relies on using ansatz states that one hopes are simple enough to compute with, yet sophisticated enough to capture important phenomena. In this work we consider one such approach — the so-called PEPS ('projected entangled pair states') formalism for a spin lattice [1]. In the PEPS formalism, an underlying lattice of pairwise-entangled 'virtual' particles is 'projected' at each site to give the final multiparticle entangled ansatz state. The use of entangled 'virtual bonds' brings complexity to the description, while helping to break the multiparty entanglement down into two-particle form that may be more tractable. Nevertheless, PEPS states can still be very complex. The cluster state of measurement based quantum computation is an example of a PEPS state [2], so sampling the outcomes of local measurements on PEPS states can be classically difficult.

In this work [3] we use the PEPS formalism for the simulation of quantum systems, but in the context of *generalised* entanglement that has arisen in the foundations of quantum theory [4]. A quantum state of two or more particles is said to be (quantum) entangled if it cannot be written as a probabilistic mixture of products of local operators drawn from the set of single particle quantum states. However, in some contexts (particularly involving restricted measurements), one may consider allowing the local operators to be drawn from a non-quantum set of operators (the dual space of the restricted measurements) other than the set single particle quantum states. In such situations states that are entangled in the quantum setting may become separable from such a generalised perspective [5]. If an operator has a separable decomposition w.r.t to a set S, we say that the operator is *S-separable*.

The above observation naturally leads to the following question: if we treat the quantum entangled virtual bonds in the PEPS formalism as separable states with respect to some non-quantum state space, then is it possible to exploit this separability in order to improve the current classical simulation techniques or provide alternative classical descriptions (such as local hidden variable models) for some PEPS states?

We suppose that the many-particle quantum state consists of d level particles arranged on a lattice, and that the lattice sites are all of degree v. The PEPS formalism allocates a 'virtual' quantum particle of D-levels to either end of each edge on the lattice, such that the two particles corresponding to each edge are in a maximally entangled state $|D\rangle$. The ansatz for the state (of the d-level particles) is then obtained by applying a linear transformation A taking the v virtual particles at each site (which live on $\mathbb{C}_D^{\otimes v}$) into a real particle at that site (living on $\mathbb{C}_d$). Collectively this gives a final (unnormalised) quantum state for the whole lattice from which we may try to calculate properties of

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interest. The parameter D is known as the 'bond-dimension', and in a typical application one tries to approximate the state of a quantum many-body system while trying to keep D as low as possible.

Our method for constructing classical models for PEPS states will rely upon the use of non-quantum state spaces to make both the virtual bonds and the physical state separable. We need one generalised state space for the D level virtual particles, denoted V, and one generalised state space for the 'real' d level particles, denoted R. The state space R is chosen to be the dual of a restricted set M of single particle quantum measurements that we are allowed to make on the d level particles, whereas V is chosen to be the *smallest* set for which the maximally entangled virtual pairs $|D\rangle$ are V-separable meaning they may be written as

$$|D\rangle\langle D| = \sum_j p_j \rho_A^j \otimes \rho_B^j \tag{1}$$

where ρ_A^j and ρ_B^j are drawn from the convex sets V_A and V_B with $V = (V_A, V_B)$, and p_j forms a probability distribution. Using the 2-norm as a notion of set size, we prove that the smallest V has at least D^2 operators [6].

Theorem 1 Consider any convex sets of operators V_A, V_B (not necessarily Hermitian or of unit trace) satisfying $||V_A||_2, ||V_B||_2 \leq \sqrt{D}$ for which $|D\rangle = \frac{1}{\sqrt{D}} \sum_j |jj\rangle$ is (V_A, V_B)-separable. Then the following must hold: (a) V_A, V_B must contain at least D^2 operators with 2-norm $\sqrt{D}$, and (b) any (V_A, V_B)-separable decomposition of $|D\rangle$ must involve only operators with 2-norm equal to $\sqrt{D}$. Finally, (c) given an operator basis consisting of D^2 orthogonal operators of 2-norm $\sqrt{D}$, the convex hull of the basis operators provides such a set, and (d) all such convex sets cannot be made strictly smaller while maintaining $|D\rangle$ separability.

Fixing D to be prime, we can explicitly find a basis of D^2 Hermitian operators of unit-trace corresponding the phase point operators that arise in the study of discrete Wigner function [7].

We now discuss how V and R can be used to write down classical models for some PEPS states. Consider a PEPS state defined by linear transformation A acting upon the virtual particles at each lattice site with degree v. If the linear transformation A satisfies

$$\mathrm{tr}\{A(V^{\otimes v})\} > 0, \quad \frac{A(V^{\otimes v})}{\mathrm{tr}\{A(V^{\otimes v})\}} \in R \tag{2}$$

for all V operators appearing in equation (1), then this means that the PEPS state defined by A is R-separable. This can be seen as follows. As we have chosen the state space V such that the virtual bonds are separable, the virtual quantum state Ψ_V can be represented as

$$\Psi_V = \sum_i p_i C_i \tag{3}$$

where the p_i are probabilities and the C_i are products of operators from V, then we can rewrite the PEPS transformation as (abusing notation slightly to now let A be the transformation on the whole lattice):

$$\Psi_V \to \Psi = \sum_i \frac{p_i \mathrm{tr}\{A(C_i)\}}{\mathrm{tr}\{A(V)\}} \frac{A(C_i)}{\mathrm{tr}\{A(C_i)\}} = \sum_i q_i W_i \tag{4}$$

where we have defined:

$$q_i := \frac{p_i \mathrm{tr}\{A(C_i)\}}{\mathrm{tr}\{A(C_i)\}} \quad W_i := \frac{A(C_i)}{\mathrm{tr}\{A(C_i)\}} \tag{5}$$

If conditions (2) are satisfied by A then the q_i will form a positive probability distribution and the W_i will be products of operators from R, hence ensuring that Ψ is R-separable. At the very least this would mean that Ψ has a local hidden variable model for measurements from M. Moreover, if it is possible to efficiently sample the classical probability distribution q_i, then because the W_i are products of operators from R, it will be possible to efficiently sample the outcomes of measurements from M on Ψ. These characteristics can in principle hold even if Ψ allows quantum computation with measurements outside M. The following recipe demonstrates that we *can* obtain multipartite quantum entangled states which are R-separable.

Recipe 2: Let $|\phi\rangle$ be a pure quantum state that is strictly from the interior of the convex set R and define the rank-1 Kraus operator $Q = |\phi\rangle\langle mmm...|$. Recall that the C_i in equation (3) are products of single virtual particle states and the $|m\rangle$ are chosen to have strictly positive overlap with each single one. Then Q is a rank-1 operator whose corresponding CP map *strictly* satisfies the conditions (2). Hence by continuity we may pick a rank > 1 Kraus operator Q' to be a small perturbation of Q, such that the corresponding CP map strictly satisfies the conditions (2). As Q' is a Kraus operator of rank > 1 the PEPS state will be a pure entangled quantum state. However, as it is also R-separable it will have a local hidden variable model w.r.t. M ■

This argument may not seem totally satisfying, as the PEPS states it creates seem to be close to product states. However, note that the argument works for any lattice shape and size, extending to an arbitrarily large number of particles. Could it hence still be possible for such a state to contain high enough many-particle quantum entanglement to do e.g. quantum computation, or have an infinite localisable entanglement length? We have not been able to answer this, but see e.g. [8] for 'almost' product pure quantum states that are universal for quantum computation.

The difficulty of resolving such questions may be a consequence of being too general, by trying to provide a single recipe that works for all R. However, for specific choices of R it is possible to find examples that illustrate a significant difference between quantum and non-quantum entanglement. Consider for instance the example of a PEPS state with a trivial identity projector. Each site is hence a quantum particle of D^v levels. Using entanglement swapping this state has infinite entanglement length. For most lattices the state would be universal for quantum computation using appropriate local measurements. However, if the allowed measurements M are restricted to Pauli measurements on each D-level subsystem at each site, then the system is R-separable. While this may seem like a trivial example, it demonstrates that even for tomographically complete sets of measurements at each site, there is no reason to expect that R-separability should imply that the state will not contain powerful forms of entanglement.

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