Optimal detection of entanglement in Greenberger-Horne-Zeilinger states

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We present a broad class of *N*-qubit Greenberger-Horne-Zeilinger (GHZ)-diagonal states such that nonpositivity under the partial transpose operation is necessary and sufficient for the presence of entanglement, including many naturally arising instances such as dephased GHZ states. Furthermore, our proof directly leads to an entanglement witness which saturates this bound. The witness is applied to thermal GHZ states to prove that the entanglement can be extremely robust to system imperfections.

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Introduction. Multipartite entanglement is still a phenomenon that is poorly understood and categorized. For some types of entangled states, such as *N*-qubit Greenberger-Horne-Zeilinger (GHZ) states, it requires very little noise (loss of a single qubit) to entirely destroy the entanglement, whereas others, such as error-correcting codes, seem much more robust. If we are ever to use entanglement as a resource in information-processing protocols, it is essential to understand when entanglement is present in a system and how to detect it. For instance, the ability of entanglement to persist at high temperatures could vastly reduce experimental requirements and has a direct bearing on the possibility of constructing quantum memories [1].

Attempts to characterize and detect multipartite entanglement are certainly not new [2–10]. Many additional references are contained in the wide-ranging review of [9]. While these strategies are capable of detecting some entanglement, the majority, with some notable exceptions, including [2–5], are unable to convey how well these characterizations perform. They might detect some entanglement, but how much is missed? Optimality results are crucially important.

A reasonable starting point for these studies is to consider classes of states, such as those that are diagonal in the GHZ basis, which arise frequently in quantum information, and are hence likely to be of most interest. Some partial categorizations are already known. For instance, thermal GHZ states can be distilled (using only local operations with respect to the full multipartite structure) up to a finite temperature, and this temperature is tight; i.e., above that temperature, entanglement cannot be distilled [4,5]. However, there is still (bound) entanglement present in these models above the distillation threshold [6]. Dür and Cirac [3] also considered a subset of GHZ-diagonal states and showed necessary and sufficient conditions for distillation and separability; for distillation of this subset, the state should be nonpositive with respect to the partial transpose (NPT) operation across every possible bipartition, whereas for full separability, the state should be positive with respect to the partial transpose (PPT) across all possible bipartitions.

In this Rapid Communication, we substantially broaden the class of GHZ-diagonal states for which the PPT condition is necessary and sufficient for the state to be fully separable. This class includes the special cases of the thermal state studied in [4–6] and the GHZ-diagonal states in [3]. Our formalism instantly yields an entanglement witness for optimally detecting that entanglement. Recent work [11] relaxes the restriction on the class of states, incorporating cluster states and error-correcting codes, at the cost of specializing the noise models considered.

GHZ-diagonal states. Consider a system of *N* qubits, and define the mutually commuting stabilizer operators

$$K_{n} = \begin{cases} X_{1} \prod_{m=2}^{N} Z_{m}, & n = 1, \\ Z_{1} X_{n}, & n \ge 2. \end{cases}$$

 X_n is the Pauli X matrix applied to qubit n, and Z_x denotes the application of Z rotations to all qubits for which the N-bit string x is 1; i.e., writing the *n*th bit of $x \in \{0,1\}^N$ as x_n ,

$$Z_x = \prod_{n=1}^N Z_n^{x_n}.$$

 K_x is similarly defined in terms of the K_n . Denoting $(|0\rangle \pm |1\rangle)/\sqrt{2}$ by $|\pm\rangle$, the +1 eigenstate of each of these stabilizers is

$$|\psi\rangle = |0\rangle|+\rangle^{\otimes(N-1)} + |1\rangle|-\rangle^{\otimes(N-1)},$$

and $|\psi_x\rangle = Z_x |\psi\rangle$ for $x \in \{0,1\}^N$ is an eigenstate of all products of stabilizers K_y with eigenvalue $(-1)^{x \cdot y}$. This is locally equivalent to other GHZ bases, which does not affect the entanglement structure that we are investigating. However, this particular formulation will allow an immediate translation of many of our results to the more general case of graph states [11]. Any state

$$\rho = \frac{1}{2^N} \sum_{y \in \{0,1\}^N} s_y K_y \tag{1}$$

is diagonal in this basis, and it is this class of states which we consider. In order for ρ to be a valid state, we require $s_0 = 1$ and $\min_{x \in \{0,1\}^N} \sum_y s_y (-1)^{x \cdot y} \ge 0$ (i.e., the eigenvector with minimum eigenvalue is nonnegative).

We are now interested in evaluating the partial transpose criterion on this state in a first step to determine when there is entanglement present in the state. Starting from Eq. (1), we introduce a bipartition $z \in \{0,1\}^{N-1}$ and take the partial transpose on those qubits on the $z_n = 1$ side. Without loss of generality, qubit 1 is assumed to be on the 0 side of the

bipartition. Recall that under the partial transpose, the Pauli operators alter by $Z_n \mapsto Z_n$, $X_n \mapsto X_n$ but $Y_n \mapsto (-1)^{z_{n-1}}Y_n$. Thus,

$$\rho^{PT} = \frac{1}{2^N} \sum_{y \in \{0,1\}^N} s_y K_y (-1)^{y_1 \sum_{n=2}^N y_n z_{n-1}}.$$

Observe that products of stabilizers remain as products of stabilizers, and as a result, the eigenvectors of ρ^{PT} are just $|\psi_x\rangle$, with eigenvalues $f_{x,z}(\vec{s})/2^N$:

$$f_{x,z}(\vec{s}) = \sum_{y \in \{0,1\}^N} (-1)^{x \cdot y} s_y (-1)^{y_1 \sum_{n=2}^N y_n z_{n-1}}.$$

If there exists an x and z such that $f_{x,z}(\vec{s}) < 0$, the state is entangled due to being NPT across the bipartition z.

Entanglement witnesses saturating PPT. Using this formalism, it is straightforward to find an entanglement witness that will saturate the PPT threshold for any state which is diagonal in the GHZ state basis. To do this, we measure the observables

$$W_{x,z} = \sum_{y \in \{0,1\}^N} (-1)^{x \cdot y} (-1)^{y_1 \sum_{n=2}^N y_n z_{n-1}} K_y.$$

For any arbitrary density matrix ρ with GHZ stabilizer expectation values \vec{s} ,

$$\operatorname{Tr}(W_{x,z}\rho) = \sum_{y \in \{0,1\}^N} (-1)^{x \cdot y} (-1)^{y_1 \sum_{n=2}^N y_n z_{n-1}} s_y = f_{x,z}(\vec{s}).$$

Hence, for GHZ-diagonal states, this gives the eigenvalues of the partial transpose of the state about bipartition *z*, and finding $\text{Tr}(W_{x,z}\rho) < 0$ for any *x* or *z* proves it is entangled. This is a genuine entanglement witness in that, for any state $\rho = \sum_{x,y} \mu_{x,y} |\psi_x\rangle \langle \psi_y |$, which may not be diagonal in the graph state basis, finding one of the observables to be negative witnesses the fact that it is entangled. To prove this, note that any ρ can be converted, via local probabilistic operations, into a graph diagonal state $\rho_d = \sum_x \mu_{x,x} |\psi_x\rangle \langle \psi_x |$ with the same diagonal elements [12] and, hence, the same values of \vec{s} . So, if ρ is fully separable, it will have the same value of $\text{Tr}(W\rho)$ as ρ_d , which we know will be positive since the local conversion to a diagonal state cannot introduce entanglement.

Separability. We are able to determine whether a GHZdiagonal state is NPT with respect to some bipartition and have an observable that can witness the entanglement. We will now study the converse, when the state is certainly not entangled. Again, the stabilizer formalism is immensely helpful. We will say that K_x and K_y have a *compatible basis* if at every site n when K_x is a Pauli matrix σ , then K_y is either σ or $\mathbb{1}$ at that site and vice versa. Such cases are relevant because each product of stabilizers K_x is just a tensor product of Pauli operators, and hence, its eigenvectors are product states. Two terms K_x and K_{v} have a simultaneous product state decomposition if they have a compatible basis. So, in order to give a fully separable decomposition of ρ , we group all terms that have a compatible basis and find the smallest eigenvalue. This grouping of terms has to have some component of the 1 added such that the minimum eigenvalue is 0. If we do this, then that grouping of terms is a separable state, with a decomposition specified by the common product basis. We are finally left with a condition that the excess weight of 1 terms should be positive. In the case of a GHZ-diagonal state, the terms K_y for $y \in \{0,1\}^N$ with $y_1 = 1$

do not have any compatible terms, whereas all terms K_y with $y_1 = 0$ are mutually compatible. We hence change notation

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$$\rho = g(\vec{s})\mathbb{1} + \sum_{y \in \{0,1\}^{N-1}} |s_{1y}| [\mathbb{1} + \operatorname{sgn}(s_{1y})K_{1y}] + \left(\sum_{y} s_{0y}K_{0y} - \mathbb{1} \min_{x \in \{0,1\}^{N-1}} \sum_{y} s_{0y}(-1)^{x \cdot y}\right)$$

slightly to K_{1y} and K_{0y} , respectively, for $y \in \{0,1\}^{N-1}$. The

decomposition therefore takes the form

Thus, provided

$$g(\vec{s}) = \left(\min_{x} \sum_{y \in \{0,1\}^{N-1}} s_{0y} (-1)^{x \cdot y} - \sum_{y \in \{0,1\}^{N-1}} |s_{1y}| \right) \ge 0$$

we have a separable decomposition of ρ . Compare this to $f_{x_0\tilde{x},\tilde{x}\oplus\tilde{z}}(\tilde{s})$ where $(-1)^{x_0} = -\text{sgn}(s_{100\dots 0})$,

$$\sum_{y \in \{0,1\}^{N-1}} s_{0y}(-1)^{\tilde{x} \cdot y} - \operatorname{sgn}(s_{100\dots 0}) \sum_{y \in \{0,1\}^{N-1}} s_{1y}(-1)^{\tilde{z} \cdot y}.$$

The two are equal if \tilde{x} corresponds to the minimal choice in the separable state decomposition, and there exists a $\tilde{z} \in \{0,1\}^{N-1}$ such that

$$\operatorname{sgn}(s_{100\dots 0})s_{1y}(-1)^{\tilde{z}\cdot y} \ge 0 \quad \forall y \in \{0,1\}^{N-1}.$$
 (2)

(If $s_{100...0} = 0$, then x_0 remains a free parameter.) If this simple condition is satisfied, then PPT exactly detects the transition between the existence of bipartite entanglement and full separability of the state which, in turn, makes our entanglement witnesses optimal.

Equation (2) gives a sufficient condition for the coincidence of thresholds for full separability and PPT. If not satisfied, is there really a separation between the PPT threshold and the best known separable state? For a three-qubit GHZ-diagonal state, Eq. (2) is fulfilled provided

$$\prod_{y\in\{0,1\}^2}s_{1y}\geqslant 0.$$

One can see that approximately half of the parameter space $\{s_y\}$ is covered by Eq. (2) in this case. One example outside this regime is the state

$$\rho = \frac{1}{8(1+\alpha)} \left(\prod_{n=1}^{3} (\mathbb{1} + K_n) - 2K_1 K_3 + \alpha \mathbb{1} \right).$$

Provided $\alpha \ge 2$, ρ is a valid state, but it is also PPT with respect to all possible bipartitions. Our previous construction of a separable state is valid for $\alpha \ge 4$. This can be improved to $\alpha \ge 2\sqrt{2}$ by rewriting the sum $K_1 + K_1K_2 - K_1K_3 + K_1K_2K_3$ as

$$\frac{1}{2}\sum_{n=0}^{1} (X+(-1)^n Y)_1 (Z+(-1)^n Y)_2 (Z-(-1)^n Y)_3.$$

Upon implementing the semidefinite programming techniques of [13], we witnessed entanglement in the region $\alpha \leq 2.828$. Hence, the separable decomposition is not universally optimal, but neither is the PPT condition.

Thermal states and perturbations. Many noise models satisfy Eq. (2), including the subclass considered in [3] (all

 s_{1y} equal and positive). We will now discuss the special case of local dephasing noise on each qubit, which also corresponds to the thermal state of the Hamiltonian

$$H = -\frac{1}{2} \sum_{n=1}^{N} \Delta_n K_n$$

which has $s_y = \prod_{n=1}^{N} \tanh(\beta \Delta_n/2)^{y_n}$, where β is the inverse temperature and Δ_n are energy terms. Since $s_y > 0$, $\tilde{z} = 00...0$. One can also check that \tilde{x} is 11...1 and, consequently, derive a simple threshold condition,

$$\tanh\left(\frac{1}{2}\beta\Delta_1\right) = e^{-\beta\sum_{n=2}^N\Delta_n}$$

Even though distillable entanglement only persists to a finite temperature [4,5], bound entanglement, which is all bipartite and detected by the partial transpose, persists to a temperature that increases with N (see Fig. 1). Without knowledge of the optimal solution, as derived here, it was impossible for previous studies of entanglement witnesses, even those specifically designed to detect GHZ state entanglement, to evaluate how well they performed, and they were often far from optimal. It is not our purpose to reevaluate the plethora of witnesses available, and instead, we merely compare one example, taken from [6]; see Fig. 1. As observed numerically for other graph states in [14], the entanglement is very robust to perturbations in the Δ_n (on qubits 2 to N, only the average dephasing strength is relevant). We can also add a local magnetic field term

$$H = -\frac{1}{2} \sum_{n=1}^{N} \Delta_n K_n - \frac{1}{2} \sum_{n=1}^{N} \delta_n Z_n$$

Since the terms $K'_n = \Delta_n K_n + \delta_n Z_n$ mutually commute, $[K'_n, K'_m] = 0$, and $K'^2_n = (\Delta_n^2 + \delta_n^2)\mathbb{1}$,

$$\rho = \frac{1}{2^N} \prod_{n=1}^N \left(\mathbb{1} + \tanh\left(\frac{1}{2}\beta\sqrt{\Delta_n^2 + \delta_n^2}\right) K'_n \middle/ \sqrt{\Delta^2 + \delta^2} \right).$$



FIG. 1. (Color online) Comparison of the PPT critical temperature for the thermal GHZ state, a lower bound for the model when perturbed by a uniform magnetic field of strength $\delta/\Delta = 0.3$, and performance comparison of a previous entanglement witness [6]. Choice of $\Delta = k_B = \hbar = 1$ ensures unitless quantities.

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For simplicity of notation, we take all the Δ_n to be equal and all the δ_n to be equal. We also set $s = \tanh(\beta \sqrt{\Delta^2 + \delta^2}/2)$. The thermal state can be expanded as

$$2^{N}\rho = \sum_{x \in \{0,1\}^{N}} \sum_{y \in \{0,1\}^{N}} \left(\frac{s}{\sqrt{\Delta^{2} + \delta^{2}}}\right)^{w_{x}+w_{y}} \delta^{w_{x}} \Delta^{w_{y}} Z_{x} K_{y},$$

although the summation over *y* is restricted to cases where $y_n = 0$ if $x_n = 1$. w_x is the Hamming weight of the string *x*. To prove the presence of entanglement, we can use the entanglement witness $W_{\tilde{x}, \tilde{x} \oplus \tilde{z}}$ from the unperturbed case,

$$\operatorname{Tr}(W_{\tilde{x},\tilde{x}\oplus\tilde{z}}\rho) = \sum_{y\in\{0,1\}^N} \left(\frac{-s\Delta}{\sqrt{\Delta^2 + \delta^2}}\right)^{w_y} (-1)^{y_1\sum_{n=2}^N y_n z_{n-1}},$$

since $\text{Tr}(Z_x K_y K_z) = \delta_{x,00...0} \delta_{y,z}$. The critical inverse temperature β_{δ} at which the expectation value of this state is zero is hence related to the unperturbed β_0 by

$$\frac{\Delta}{\sqrt{\Delta^2 + \delta^2}} \tanh\left(\frac{1}{2}\beta_\delta\sqrt{\Delta^2 + \delta^2}\right) = \tanh\left(\frac{1}{2}\beta_0\Delta\right).$$

Furthermore, β_{δ} is an upper bound on the true critical β , i.e., a lower bound on the critical temperature. Figure 1 indicates just how robust this entanglement is.

Approximate entanglement witnesses. With the advent of an optimal solution to the detection of GHZ-like entanglement, we come across the problem that the desired entanglement witness is composed of exponentially many terms. This is to be expected since, in order to function over such a wide parameter regime, it will be necessary to take into account the fine detail of the exponentially many parameters of the state. Nevertheless, one can study how to approximate these witnesses, and we advocate the approach of starting from the optimal solution. Figure 2 shows how to implement an additive approximation to the witnesses across the entire parameter regime. For any $\rho = \sum_{a,b} \mu_{b,a} |\psi_b\rangle \langle \psi_a |$, the first two gates are just the sequence that maps $|\psi_a
angle$ into a computational basis state $|a\rangle$, so this circuit simply represents the input of a state $\sigma = (\sum_{a,b} \mu_{b,a} | b \rangle \langle a |) \otimes \mathbb{1}/2^N$ to a Hadamard test using a 2N-qubit unitary V. The Hadamard test has a probability of finding the ancilla in state $|0\rangle$ of $\frac{1}{2}(1 + \operatorname{Tr}(\sigma V))$. It is readily verified that $\operatorname{Tr}(\sigma V) = \operatorname{Tr}(W_{x,z}\rho)$. After k repetitions, the probability of incorrectly estimating the value of $Tr(W_{x,z}\rho)$ to an accuracy ε is bounded by Chernoff's bound to be no worse than $2e^{-2k\varepsilon^2}$, so using $k \sim O(\varepsilon^{-2})$ gives a constant failure probability, independent of N, with a number of gates O(N). Further details can be found in [11].



FIG. 2. Circuit for additive approximation to optimal entanglement witnesses. The top register is a single ancilla. The other two are registers of *N* qubits. Gates are applied transversally, except for CP_E , which indicates that controlled phases need to be applied between the qubits of a given register for all pairs (1,n). CP_E^z is similar except that the controlled phase between qubits 1 and *n* is only applied if $z_n = 1$.

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Let us now consider witnessing entanglement for thermal states. With the promise that a state is a thermal GHZ state, it is only necessary to measure the value of s because we know the critical value. However, the trick is to build this added simplicity into a witness. If we start from an N-qubit thermal GHZ state, we could apply controlled-phase gates along all qubit pairs (1,n). This would return a state where every qubit is in a separable state $|+\rangle\langle+|+s|-\rangle\langle-|$, from which we could easily extract s, although this is not a witness. However, if we only measured a subset, M, of the N qubits, we could invoke the quantum De Finetti theorem [15], which states that to an approximation that scales with M/(N - M), the M qubits can be found in a separable state $\int d\sigma p(\sigma) \sigma^{\otimes M}$, where $p(\sigma)$ is some probability distribution over all possible single-qubit states σ (except that in the present case they must be diagonal in the $|\pm\rangle$ basis), each of which corresponds to a thermal state parametrized by $s(\sigma)$. By measuring several copies of this state, it is possible to approximate $p(\sigma)$ and hence witness if the state is entangled by evaluating $\int d\sigma p(\sigma) f_{x,z}(s(\sigma))$. If the subset of M qubits was entangled, the full set of N qubits certainly was. The entanglement lost by tracing out a large proportion of the qubits will negatively impact the optimality, particularly for GHZ states, but for other states, such as the onedimensional cluster state [11], this approximation is very mild.

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Conclusions. We have given a sufficient condition, which naturally encompasses a vast range of GHZ-diagonal states, including those that are experimentally relevant, such that the existence of an NPT bipartition is necessary and sufficient for the state to be entangled. This led to an entanglement witness that optimally detects the existence of an NPT bipartition and shows that the entanglement in thermal states of GHZ graphs is extremely robust to some classes of perturbation. Future work could focus on witnessing entanglement in those cases where entanglement persists outside the PPT regime, beyond the current reliance on numerical techniques. Criteria developed in [10] can already prove the existence of entanglement beyond the PPT threshold.

We have been careful to express much of this Rapid Communication in very general terms using the stabilizer formalism. As such, much of the work extends to graphdiagonal states, which are also defined by stabilizers and which cover many of the interesting states in quantum information, such as cluster states and error-correcting codes. We study this case in more detail in [11].

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