Bound Genuine Multisite Entanglement: Detector of Gapless-Gapped Quantum Transitions in Frustrated Systems

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We define a multiparty entanglement measure, called generalized geometric measure, that can detect and quantify genuine multiparty entanglement for any number of parties. The quantum phase transitions in exactly solvable models like the anisotropic XY model can be detected by this measure. We find that the multisite measure can be a useful tool to detect quantum phenomena in more complex systems like quasi 2D and 2D frustrated Heisenberg antiferromagnets. We propose an order parameter, called bound generalized geometric measure, in the spirit of bound quantum states, that can recognize the gapless and gapped phases of the frustrated models by its sign. The vanishing of the order parameter therefore signals the transition between such phases.

I. INTRODUCTION AND MAIN RESULTS

The rapid development of the theory of entanglement over the last decade or so [1], and its usefulness in communication systems and computational devices, as well as the experimental observations of entangled states in a variety of distinct physical systems [2], have attracted a lot of attention from different branches of physics, including condensed matter and ultra-cold gases [3, 4]. It has been argued that entanglement can be used as a "universal detector" of quantum phase transitions, with most of the studies being on the behavior of *bipartite* entanglement [5, 6]. A more natural way to study the many-body systems would be to consider multipartite entanglement, as almost all naturally occurring multisite quantum states are genuinely multi-party entangled. Such an enterprise is however limited by the intricate nature of entanglement theory in the multisite scenario. In particular, only a few multisite entanglement measures are known, and moreover their computation are difficult [1].

Multipartite states can have different hierarchies according to their entanglement quality and quantity. The simplest example is for three-particle states, where there are fully separable, biseparable, and genuine multipartite entangled states. A measure of genuine multiparty entanglement, quantifies, so to say, the "purest" form multiparty entanglement. In this paper, we define an entanglement measure, called generalized geometric measure (GGM), that can detect and quantify genuine multiparticle entanglement. Interestingly, the measure is computable for arbitrary pure states of multiparty systems in arbitrary dimensions and arbitrary number of parties, and therefore can turn out to be a useful tool to detect quantum many-body phenomena, like quantum phase transitions. In this respect, GGM has the potential of gaining the same status in applications of multiparty entanglement theory, as that of logarithmic negativity [6] in the bipartite domain.

As an initial testing ground, we use the GGM to successfully detect quantum phase transitions in the anistropic XY model on a chain of spin-1/2 particles [7]. Our main aim however is to apply the measure to states of frustrated spin systems, for which the phase diagrams are not exactly known. Frustrated many-body systems are a center of interest in condensed matter physics due to the typically rich and novel phase diagrams in such systems. Moreover, experimental realizations of many metal oxides, including those exhibiting high-Tc superconductivity, typically have frustrated interactions in their Hamiltonians [8, 9]. As paradigmatic representatives of such systems, we consider (i) the quasi 2D antiferromagnetic $J_1 - J_2$ Heisenberg model with nearest neighbor couplings, J_1 , and next-nearest neighbor couplings, J_2 [10–12], and (ii) the frustrated $J_1 - J_2$ model on a square lattice [8] (see Fig. 1).



FIG. 1: (Color online.) Two-dimensional $J_1 - J_2$ model, with vertical and horizontal couplings, J_1 , and diagonal couplings, J_2 The predicted phase diagram is also schematically shown.

For studying such systems, we introduce an order parameter which is the difference between the GGM (\mathcal{E}) and its second derivative with respect to the system parameter, μ , that drives the transitions in the system. We call the quantity as "bound GGM", and is given by

$$\mathcal{E}_B \equiv \mathcal{E} - \frac{d^2 \mathcal{E}}{d\mu^2}$$

The ground state manifold of the quasi 2D $J_1 - J_2$ system is not known exactly, except at the Majumdar-Ghosh point [10], i.e. for $\alpha = J_2/J_1 = 0.5$, where the system is highly frustrated, and presents two dimer states as its ground states. However, exact diagonalization and group theoretical studies show that the system is gapless, and hence critical, in the weakly frustrated regime, namely $0 \le \alpha \lesssim 0.24$ [10, 11]. For higher coupling ratio α , the

system enters a dimerized regime, and is gapped [10, 13]. We study the GGM for this system by exact diagonalization, and show that the bound GGM vanishes at the fluid-dimer transition point $\alpha \approx 0.24$. Note here that it is known that bipartite entanglement cannot detect the gapless phase [14] (cf. [15]). We find that the bound GGM is positive in the gapless phase while it becomes negative in the gapped one. The Majumdar-Ghosh point can also be detected by the GGM.

Finally we apply our measure of genuine multisite entanglement to the ground state of the 2D Heisenberg system. As depicted in Fig. 1, the Néel and collinear ordered phases (the gapless phases dissociated by a phase having a finite gap between the singlet ground state and the excited states. We show that the bound GGM can detect both the quantum phase transitions – from the Néel phase to the dimerized one at $\alpha \approx 0.38$, as well as the transition from the dimer to the collinear phase at $\alpha \approx 0.69$, as predicted, even for relatively small systemsize. Like in the $J_1 - J_2$ ring, the positivity (negativity) of the bound GGM indicates the gapless (gapped) phase.

Armed with these findings, we propose that the bound GGM can potentially be used for detecting gapped/gapless phases in many-body systems:

$$\mathcal{E}_B > 0 \Rightarrow \text{gapless}, \quad \mathcal{E}_B < 0 \Rightarrow \text{gapped}.$$
 (1)

This leads to an analogy with the thermodynamics of bound entanglement [1, 16]. Analogous to the first law of thermodynamics, internal energy = free energy + work done, a thermodynamic equation of entanglement was written: Entanglement cost = distillable entanglement + bound entanglement, where the bound entanglement is the amount of entanglement necessary to keep the transition (under local quantum operations and classical communication) from becoming irreversible. As another face of this entanglement-energy analogy, a negative value of \mathcal{E}_B , assuming the thesis in Eq. (1), indicates that the system needs a nonzero amount of energy to free itself from its ground state. We hope that this can help us in a quantification of the first law of the emerging entanglement thermodynamics [1, 17]. This is the reason for calling \mathcal{E}_B as bound GGM [18].

II. GENERALIZED GEOMETRIC MEASURE

Let us begin by defining the generalized geometric measure. As mentioned above, GGM will quantify the genuineness of multiparty entanglement. An *N*-party pure quantum state is said to be genuinely *N*-party entangled, if it is not a product across any bipartite partition. The simplest examples of genuine tripartite entangled states are the Greenberger-Horne-Zeilinger [19] and W [20] states. The GGM of an *N*-party pure quantum state $|\psi\rangle$ is defined as

$$\mathcal{E}(|\psi\rangle) = 1 - \Lambda_{max}^2(|\psi\rangle), \qquad (2)$$

where $\Lambda_{max}(|\psi\rangle) = \max |\langle \phi |\psi \rangle|$, with the maximization being over all pure states $|\phi\rangle$ that are not genuinely *N*party entangled. Note that the maximization performed in GGM is different from the maximization in the geometric measure of Ref. [21] (cf. [22]).

A. Properties

Clearly, \mathcal{E} is vanishing for all pure multiparty states that are not genuine multiparty entangled, and nonvanishing for others. We considered this quantity for four-party states in Ref. [23], and showed it to be a monotonically decreasing quantity under local quantum operations and classical communication (LOCC). Applications of GGM to quantum many-body systems requires us to find its properties for an arbitrary number of parties.

Let $|\psi\rangle$ be an *N*-party pure quantum state in the tensor product Hilbert space $\mathcal{H}_{A_1} \otimes \mathcal{H}_{A_2} \otimes \ldots \otimes \mathcal{H}_{A_N}$. Therefore, the maximization in

$$\Lambda_{\max}(|\psi\rangle_{A_1A_2...A_N}) = \max_{|\phi\rangle_{A_1A_2...A_N}} |\langle\phi|\psi\rangle| \qquad (3)$$

is over all pure quantum states $|\phi\rangle_{A_1A_2...A_N}$, in $\mathcal{H}_{A_1} \otimes$ $\mathcal{H}_{A_2} \otimes \ldots \otimes \mathcal{H}_{A_N}$, that are not genuinely multiparty entangled, which is a rather large class of states. Note however, that the square of $\Lambda_{\max}(|\psi\rangle_{A_1A_2...A_N})$ can be interpreted as the Born probability of some outcome in a quantum measurement on the state $|\psi\rangle$. Now, entangled measurements cannot be worse than the product ones for any set of subsystems. Therefore, in the maximization, we do not need to consider the $|\phi\rangle_{A_1A_2...A_N}$ that are product in a partition of A_1, A_2, \ldots, A_N into three, four, ... sets. The only $|\phi\rangle_{A_1A_2...A_N}$ that are to be considered are the ones that are a product in a bipartition of A_1, A_2, \ldots, A_N . This greatly reduces the class over which the maximization is carried out. Let $\mathcal{A}: \mathcal{B}$ be such a bi-partition. Then, max $|\langle \phi | \psi \rangle|$, where the maximization is carried over the $|\phi\rangle$ that are product across $\mathcal{A} : \mathcal{B}$, is the maximal Schmidt coefficient, $\lambda_{\mathcal{A}:\mathcal{B}}$, of the state $|\psi\rangle_{A_1A_2...A_N}$ in the \mathcal{A} : \mathcal{B} bipartite split. $\Lambda_{\max}(|\psi\rangle_{A_1A_2...A_N})$ is therefore the maximum of all such maximal Schmidt coefficients in bipartite splits. Note that the λ 's involved in this closed form for Λ_{max} are all increasing under LOCC [24]. We have therefore proven the following theorem.

Theorem. The generalized geometric measure of $|\psi\rangle_{A_1A_2...A_N}$ is given by

$$\mathcal{E}(|\psi\rangle) = 1 - \max\{\lambda_{\mathcal{A}:\mathcal{B}}^2 | \mathcal{A} \cup \mathcal{B} = \{1, 2, \dots, N\}, \mathcal{A} \cap \mathcal{B} = \emptyset\}.$$
(4)

It is computable for a multiparty pure state of an arbitrary number of parties, and of arbitrary dimensions. Also, it is monotonically decreasing under LOCC.

III. ANISOTROPIC XY MODEL

The one-dimensional XY model with N lattice sites is described by the Hamiltonian

$$H_{XY} = \frac{J}{2} \left(\sum_{i=1}^{N} (1+\gamma)\sigma_i^x \sigma_{i+1}^x + (1-\gamma)\sigma_i^y \sigma_{i+1}^y \right) + h \sum_{\substack{i=1\\(5)}}^{N} \sigma_i^z$$

where J is the coupling constant, $\gamma \in [0,1]$ is the anistropy parameter, σ 's are the Pauli matrices, and hrepresents the magnetic field in the transverse direction. The quantum transverse Ising and the transverse XX models correspond to two extreme values of γ , which are resepectively $\gamma = 1$ and $\gamma = 0$. This model can be diagonalized by the Jordan-Wigner transformation [7]. Apart from its other interests, it is the simplest model which shows a *quantum* phase transition, driven by the magnetic field, at zero temperature. It is known to be detectable by using bipartite entanglement measures [25], like concurrence [5]. However, evaluating GGM will additionally quantify the nature of genuine multiparty entanglement of the ground state in this model, especially as it crosses the transition point.

The diagonalization of this model can be achieved by introducing the Majorana fermions

$$c_{2l-1} = (\Pi_{i=1}^{l-1} \sigma_i^z) \sigma_l^x; \quad c_{2l} = (\Pi_{i=1}^{l-1} \sigma_i^z) \sigma_l^y. \tag{6}$$

The Hamiltonian in Eq. (5) thereby reduces to a quadratic fermionic Hamiltonian [7]. The eigenvalues of the reduced density matrix of L sites of the ground state of this system can be obtained by using the above formalism [4], and is given by

$$e_{x_1x_2\dots x_l} = \prod_{i=1}^{L} \frac{1 + (-1)^{x_i} \nu_i}{2}, \quad x_i = 0, 1 \; \forall i, \qquad (7)$$

where ν_i 's are the eigenvalues of G_L , which in turn is given by $B_L = G_L \otimes \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}$, with

$$G_L = \begin{bmatrix} g_0 & \cdot & g_{L-1} \\ \cdot & \cdot & \cdot \\ -g_{L-1} & \cdot & g_0 \end{bmatrix}, B_L = \begin{bmatrix} \Pi_0 & \cdot & \Pi_{L-1} \\ \cdot & \cdot & \cdot \\ -\Pi_{L-1} & \cdot & \Pi_0 \end{bmatrix}$$

Here, $\Pi_l = \begin{bmatrix} 0 & g_l \\ -g_{-l} & 0 \end{bmatrix}$, and the real coefficients, g_l , are given by

$$g_l = \frac{1}{2\pi} \int_0^{2\pi} d\phi e^{-il\phi} \frac{\cos\phi - \lambda - i\gamma\sin\phi}{|\cos\phi - \lambda - i\gamma\sin\phi|}, \qquad (8)$$

where $\lambda = J/h$.

The derivative of GGM of the ground state, for different anistropy parameters γ , clearly shows a logarithmic divergence at the transverse field given by $\lambda = 1$, as seen in Fig. 2. Note also that the ground state of the transverse Ising model ($\gamma = 1$) has higher genuine multipartite entanglement as compared to the ground states for other values of γ . This result may help us to understand the success of the dynamical states of the transverse Ising model as a substrate for efficient quantum computation [26].



FIG. 2: (Color online.) GGM of the transverse XY model. The GGM (actually $\mathcal{E} - 1/2$) and its derivative (both dimensionless) are plotted on the vertical axis for the anistropic transverse XY model for different anisotropy parameters γ , against the dimensionless system parameter λ on the horizontal axis. The dashed (blue), circled (pink), and dotted (green) lines are respectively for the Ising ($\gamma = 1$), $\gamma = 0.8$, and $\gamma = 0.2$ models. The derivatives of GGM diverges at the quantum critical point $\lambda = 1$.

IV. QUASI 2D FRUSTRATED $J_1 - J_2$ MODEL

We will now consider the frustrated quasi twodimensional $J_1 - J_2$ Heisenberg model, in the case when both the nearest neighbor couplings, J_1 , and the nextnearest neighbor couplings, J_2 , are antiferromagnetic. Apart from its other interests, the intense interest for studying this model lies in the fact that it is similar to real systems, like SrCuO₂ [27]. The Hamiltonian of this model, with N lattice sites on a chain, is

$$H_{1D} = J_1 \sum_{i=1}^{N} \vec{\sigma}_i \cdot \vec{\sigma}_{i+1} + J_2 \sum_{i=1}^{N} \vec{\sigma}_i \cdot \vec{\sigma}_{i+2}, \qquad (9)$$

where J_1 and J_2 are both positive, and where periodic boundary condition in assumed. The ground state and the energy gap of this model were studied by using exact diagonalization, density matrix renormalization group method, bosonization technique, etc [12]. For an even number of sites, the ground state at the Majumdar-Ghosh point ($\alpha = J_2/J_1 = 0.5$), is doubly degenerate, and the ground state manifold is spanned by the two dimers $|\psi_{MG}^{\pm}\rangle = \prod_{i=1}^{N/2} (|0\rangle_{2i}|1\rangle_{2i\pm 1} - |1\rangle_{2i}|0\rangle_{2i\pm 1})$, and the model is gapped at this point [10]. For $\alpha = 0$, the Hamiltonian reduces to the s = 1/2 Heisenberg antiferromagnet and hence the the ground state, which is a spin fluid state having gapless excitations [28], can be obtained by Bethe ansatz. It is known that at $\alpha \approx 0.2411$, a phase transtion from fluid to dimerization occurs [29].

The genuine multipartite entanglement measure clearly signals the Majumdar-Ghosh point (See Fig. 3). The fluid-dimer tranition at $\alpha \approx 0.24$ can also be detected by the vanishing of the bound GGM as the order parameter (for $\mu = \alpha$) (see Fig. 3). Moreover, $\mathcal{E}_B > 0$ signals the gapless phase, while $\mathcal{E}_B < 0$ indicates the gapped phase.



FIG. 3: (Color online.) GGM and bound GGM for the quasi-2D frustrated antiferromagnet. The left figure is for the GGM on the vertical axis against α on the horizontal. The Majumdar-Ghosh point at $\alpha = 0.5$ is clearly signaled. The figure on the right is for the bound GGM on the vertical axis, against α on the horizontal, and the fluid-dimer transition is signaled by the vanishing of the bound GGM. The two curves are for 8 (red circles) and 10 (blue squares) spins in both the figures. The GGM, bound GGM, and α are all dimensionless.

V. 2D FRUSTRATED $J_1 - J_2$ MODEL

We now consider spin-1/2 particles on a square lattice, where nearest neighbor spins (both vertical and horizontal) on the lattice are coupled by Heisenberg interactions, with coupling strengths J_1 , and where all diagonal spins are coupled by Heisenberg interactions, with coupling strengths J_2 (see Fig. 1). This 2D model have attracted a lot of interest [30] due to its connection with the high T_c -superconductors and its similarity with magnetic materials like Li₂VOSiO₄ and Li₂VOGeO₄ [31]. Although the different phases of the ground state of this model is well-studied, there seem to exist reasons to believe in further secrets hidden. The Hamiltonian of the system is therefore given by

$$H_{2D} = J_1 \sum_{\langle i,j \rangle} \vec{\sigma}_i \cdot \vec{\sigma}_j + J_2 \sum_{i,j \in \mathcal{D}} \vec{\sigma}_i \cdot \vec{\sigma}_j.$$
(10)

Both J_1 and J_2 are antiferromagnetic (> 0).

In the classical limit, the model exhibits only a firstorder phase transition from Néel to collinear at α = $J_2/J_1 = 0.5$. The phase diagram changes its nature, when quantum fluctuations are present, and in this case, the exact phase boundaries are not known. It is expected that two long range ordered (LRO) ground state phases are separated by quantum paramagnetic phases without LRO. Different methods, like exact diagonalization, series expansion methods, field-theory methods [32], etc., applied to this model, predict that the first transition from Néel to dimer accurs at $\alpha \approx 0.38$ while other one happens at $\alpha \approx 0.66$. Recent experimental observations and proposals of detecting such phases in the laboratory demand the precise quantification of the phase diagram of this model at low temperature. Towards this aim, we show that even for relatively small system size, the order parameter based on the genuine multipartite entanglement measure (the \mathcal{E}_B , introduced above) can detect and quantify the phase diagram accurately.

We perform exact diagonalization to find the ground state of the model, and we show that both the transitions – Néel to dimer and dimer to collinear can be signaled by the bound GGM. A synopsis of these facts is given in Fig. 4. Precisely, we have found that \mathcal{E}_B vanishes at $\alpha \approx 0.38$ and again at $\alpha \approx 0.69$. As observed in the case of the quasi 2D $J_1 - J_2$ model, \mathcal{E}_B is positive in the gapless phases while it is negative in the intermediate gapped phase.

VI. CONCLUSIONS

Multipartite entangled states can be classified according to their separability in different partitions. Due to the complex classification, it is hard to obtain a unique multipartite entanglement measure. Instead of quantifying all the classes of multipartite states, we define an entanglement measure, called generlized geometric measure, that quantifies the "purest" form of multiparty entanglement, the genuine multipartite entanglement. This is akin to the situation in bipartite pure states, where there is essentially a unique entanglement measure, while mixed bipartite states allows a number of such measures [1]. In the case of multiparty states, we find "pure" and "nonpure" forms of entanglement, even within the class of pure states, where the "pure" part can be quantified by the generalized geometric measure defined here. Moreover, we found that the measure can be reduced to a



FIG. 4: (Color online.) GGM and bound GGM for the 2D frustrated antiferromagnet. The horizontal axes in both the figures represent α . The left figure is for the GGM on the vertical axis while the right one is for the bound GGM. The vanishing of the bound GGM signals both the Néel-to-dimer and the dimer-to-collinear transitions. And the gapped (gapless) phase(s) is (are) signaled by a negative (positive) bound GGM. The two curves are for 9 spins on a 3×3 square lattice (red circles), and 12 spins on a 3×4 rectangular lattice (blue squares) in both the figures. The GGM, bound GGM, and α are all dimensionless.

simplified closed form, and hence is computable for arbitrary dimensions and arbitrary number of parties.

We then applied this measure to detect phase diagrams in quantum many-body systems. After successfully verifying that the measure can detect quantum fluctuation driven phase transitions in the exactly solvable models like the XY Hamiltonian, we applied the generalized geometric measure to frustrated models like quasi two dimensional and two dimensional antiferromagnetic $J_1 - J_2$ models. In the latter case, the phase diagram is not known exactly, although there has been several predictions by different methods. In this paper, we show that an order parameter, called bound GGM, based on the multi-site entanglement measure defined, can signal the phase boundaries in both the models. Moreover, we found the order parameter is positive when the system is gapless and negative in the gapped phase. We propose that the sign of the bound GGM can indicate whether a many-body system is gapped or gapless, and point to its implication for the first law of entanglement thermodynamics.

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