Topological Entanglement Entropy of a Bose-Hubbard Spin Liquid

Sergei V. Isakov  
Theoretische Physik, ETH Zurich, 8093 Zurich, Switzerland

Matthew B. Hastings  
Duke University, Department of Physics, Durham, NC, 27708 and  
Microsoft Research, Station Q, CNSI Building, University of California, Santa Barbara, CA, 93106

Roger G. Melko  
Department of Physics and Astronomy, University of Waterloo, Ontario, N2L 3G1, Canada  
(Dated: January 12, 2013)

The Landau paradigm of classifying phases by broken symmetries was demonstrated to be incomplete when it was realized that different quantum Hall states could only be distinguished by more subtle, topological properties [1]. Today, the role of topology as an underlying description of order has branched out to include topological band insulators, and certain featureless gapped Mott insulators with a topological degeneracy in the groundstate wavefunction. Despite intense focus, very few candidates for these topologically ordered “spin liquids” exist.

The main difficulty in finding systems that harbour spin liquid states is the very fact that they violate the Landau paradigm, making conventional order parameters non-existent. Here, we uncover a spin liquid phase in a Bose-Hubbard model on the kagome lattice, and measure its topological order directly via the topological entanglement entropy. This is the first smoking-gun demonstration of a non-trivial spin liquid, identified through its entanglement entropy as a gapped groundstate with emergent $Z_2$ gauge symmetry.

Quantum spin liquid phases are notoriously elusive, both in experimental materials and in theoretical models. In part, this is due to the delicate balance of microscopic interaction that must occur so that conventional symmetry-broken order is suppressed to low temperatures. The search is also hampered by the lack of a measurable order parameter, such as magnetization, that would offer a positive indicator of spin liquid behavior. Instead, the current procedure of identifying spin liquids involves eliminating all possible order parameters through exhaustive searches of correlation functions [2]. Theoretical work has nonetheless developed a classification scheme of gapped spin liquid states based on the topological degeneracy of their wavefunction. In fact, there exist several model Hamiltonians that have been proposed to contain spin liquid groundstates with the most trivial $Z_2$ topological order (corresponding to a four-fold degeneracy on a torus). One of the earliest was the triangular-lattice quantum dimer model [3] – where dimers are intended to be an effective description of local singlet correlations, not physical spins. Another paradigm in studying topological order has recently emerged in the toric code [4], as it is the simplest of a class of exactly solvable models (such as the Levin-Wen models [5]) describing different topological quantum field theories. Unfortunately, these models require somewhat artificial multi-spin interaction terms.

In order for a model to be relevant for real physical systems, it is essential to find a spin Hamiltonian with simple two-body interaction terms and a topologically ordered spin liquid state. One important step in this direction occurred with the introduction of a kagome Bose-Hubbard model by Balents, Girvin and Fisher [6]. Although this model has a four-spin interaction, it contains a $Z_2$ spin liquid over an extended region of its phase diagram. Previously, a related model was shown through quantum Monte Carlo (QMC) studies to have a featureless Mott insulating state [7, 8], where, like most experimental candidates, the absence of order in correlation functions was the main evidence for spin liquid behavior.

In 2006, Levin and Wen [9] and Kitaev and Preskill [10] identified a quantity $2\gamma$ called the topological entanglement entropy (EE) which is designed to replace the concept of an “order parameter” in a topologically ordered...
system. Based on the idea that the spin liquid state is a type of collective paramagnet, the topological EE is designed to pick up non-local correlations in the ground-state wavefunction that are not manifest as conventional long-range order. However, these correlations contribute to the total entanglement between different subregions of the system $A$ and its complement $B$ (where $A \cup B$ is the entire system). The EE between $A$ and $B$ can be quantified by the Renyi entropies,

$$S_n(A) = \frac{1}{1-n} \ln [\text{Tr}(\rho_A^n)],$$

where $\rho_A$ is the reduced density matrix of region $A$. In a topologically ordered state, the non-local entanglement gives a topology-dependent subleading correction to “area-law” scaling of the EE of subregion $A$. In 2D, $S_n(A) = a\ell - \gamma j + \cdots$ where $a$ is a non-universal constant, $\ell$ is the boundary length between $A$ and $B$, and $j$ is the number of disconnected boundary curves. In Levin and Wen’s construction (used in the calculations in this paper), the topological contribution can be isolated from the area-law scaling (plus any corner contributions) by considering separately the Renyi entropies on four differently shaped subregions (Figure 1).

$$2\gamma = \lim_{r,R \to \infty} [-S_n(A_1) + S_n(A_2) + S_n(A_3) - S_n(A_4)].$$

(2)

Naively, since calculating $\gamma$ requires complete knowledge of the groundstate wavefunction (through $\rho_A$), previous efforts to calculate it have been restricted to models which can be solved exactly either analytically (e.g. the toric code) or through numerical exact diagonalization on small size systems (e.g. the triangular lattice dimer model). The ability to use $\gamma$ as a general tool to search for and characterize non-trivial topologically ordered phases has been hindered by the inability to access the wavefunction in large-scale numerical methods, namely QMC, currently the only scalable quantum simulation method in 2D and higher. However, with the recent introduction of measurement methods based on the replica trick, QMC is now able to access $S_n(A)$ for $n \geq 2$, therefore giving one a method to calculate $\gamma$ in large-scale simulations of quantum spin liquids.

Using Stochastic Series Expansion QMC, we simulate a hard-core Bose-Hubbard model on the kagome lattice, with nearest-neighbor hopping and a six-site potential around each lattice hexagon,

$$H = -t \sum_{\langle ij \rangle} [b_i^\dagger b_j + b_j b_i^\dagger] + V \sum_{\partial} (n_\partial)^2,$$

(3)

where $b_i^\dagger$ ($b_i$) is the boson creation (annihilation) operator, and $n_\partial = \sum_{i \in \partial} n_i$, where $n_i = b_i^\dagger b_i$ is the number operator. As mentioned above, variations of this model with more complicated spin interactions are known to harbour a robust spin liquid groundstate. In this paper, we consider the simplified Hamiltonian, with only nearest-neighbor hopping, which may be more amenable to construction for example in real cold atomic systems. We observe a transition at low temperature between a superfluid phase and an insulating phase for $V/t < 7.0665(15)$ (Figure 2). For $V/t > (V/T)_{c}$ the superfluid density scales to zero, and density and bond correlators are featureless (similar to Ref. 7). This strongly suggests that the insulating phase is a spin liquid. To characterize it, we calculate the topological EE, Equation (2) with $n = 2$, which for a $Z_2$ topological phase should approach $2\ln(2)$ in the limit $T \to 0$. The regions $A_i$ are shown in Figure 1 for an $L = 8$ system; these are scaled proportionally for the other system sizes studied in this paper, where $L$ is always a multiple of 8. Results for $\gamma$ as a function of inverse temperature $\beta = 1/T$ are shown in Figure 2 for several $V/t$.

In the topological phase ($V/t = 8$) we see two distinct plateaus, at differing temperatures, with a non-zero topological EE as $T \to 0$. The phenomenon is known to occur in other models such as the toric code, where the topological EE at zero temperature of $2\ln(2)$ can be viewed as a sum of electric and magnetic contributions, each contributing $\ln(2)$. If the electric and magnetic defects have different energies, theory predicts two distinct plateaus corresponding to these individual crossover temperatures, as seen in our data. However, at any fixed non-zero temperature, in the limit of large $L$, the topological EE vanishes, as the probability of having thermally excited defects in the annulus $A_1$ (Figure 1) tends to unity. Indeed, under the assumption that the probability of having a defect is proportional to $L^2 \exp(-E/k_BT)$, where $E$ is the defect energy, the temperature required to see accurate plateaus in the topological EE scales logarithmically with $L$. In Figure 3 we show finite-size scaling data consistent with this logarithmic scaling. Note that our value for the topological EE at the higher-$T$ plateau is indeed very close to $\ln(2)$, and becomes more accurately quantized at larger system sizes. The value of $2\ln(2)$ at the lower-$T$ plateau for $L = 8$ is not as accurately quantized, but is still approached.

In the superfluid phase, the topological EE tends to zero as $T \to 0$ (Figure 3). However, surprisingly, for $V/t = 6$ we observe a plateau in the topological EE at intermediate temperatures, $T \sim t$. One possible explanation for this plateau can be understood by thinking of a simpler phase transition present in the toric code, induced by adding a parallel magnetic field. Consider a square-lattice toric code Hamiltonian $H = -U \sum_i S_i^z - g \sum_i S_i^y - h \sum_i S_i^x$, where the first vertex term term penalizes vertices that do not have an even number of up spins on the legs of the neighboring bonds, and the second sum is over plaquettes. Suppose $U \gg g$. By increasing $h/g$, we induce a phase transition from a topological phase to a trivial phase. In a non-zero temperature regime where $U \gg T \gg g$, the problem be-
comes classical: the quantum dynamics induced by $g$ can be ignored and the vertex term restricts us to states described by closed loops of up spins. In this classical problem, there is a phase transition as $h/T$ increases from a topological phase with long loops to a trivial phase with only short loops (this transition is dual to the 2D Ising transition). Thus, at high temperatures (small $h/T$) we see a topological EE, while at lower $T$ the topological EE disappears. In fact, this kind of physics has been suggested to occur as a “cooperative paramagnet” in a related kagome lattice model [8].

The QMC results indicate a quantum critical point, separating the superfluid and topological phases, for a critical $V/t$ located precisely by studying the finite size scaling of the superfluid density $\rho_s$ (Figure 2). The data scales very well with the dynamical exponent $z = 1$ and the XY value for the correlation length exponent $\nu = 0.6717$ at $(V/t)_c = 7.0665(15)$. At $T = 0$ near the quantum critical point, we expect good quantization of the topological EE whenever $L$ is sufficiently large compared to the correlation length $\xi$, so the topological EE may be controlled by a scaling function of $L/\xi$. At $T > 0$, the scaling of the topological EE in the quantum critical fan appears not to have been considered previously; the plateau at intermediate temperatures for $V/t = 6$ can perhaps also be understood as a manifestation of increasing $T$ moving one from the zero temperature trivial phase into the quantum critical fan. Even at $T = 0$, the behavior of constant terms in the entropy at a critical point is largely unexplored, and may depend sensitively upon the geometry used to define it [23]. Scaling predicts that near the critical point the topological EE is a function of $\beta/\xi$ and $L/\xi$, implying that in the topological phase, corrections to $2\ln(2)$ should depend upon $(L/\xi)^2 \exp(-\beta/\xi)$, consistent with a defect energy of order $1/\xi$. Based on the intermediate temperature plateau at $V/t = 6$, it seems likely that only one type of defect, the magnetic defect, becomes gapless at criticality.

Discussion - In order to identify a topological phase, it is essential to perform non-local probes. Experimentally, such non-local probes could involve braiding operations as in the proposal of [18]. In this paper, we have shown that the topological entanglement entropy (EE), calculated by QMC using the replica trick, is a practical numerical non-local probe. Other probes might be possible, such as calculating the ground state degeneracy on lattices of different topology. However, that probe suffers from two drawbacks. First, studying surfaces of different Euler characteristic requires introducing defects, which is undesirable [23]. Second, while it would be possible in QMC to calculate the ground state degeneracy by integrating the specific heat, it requires accurate simulations at a temperature low enough to suppress all excitations - a regime where simulation ergodicity typically becomes a problem. In contrast, we have demonstrated that measurement of topological EE yields accurate quantization once one has suppressed all topologically non-trivial defects – and indeed one even sees accurate quantization at higher temperature where only one kind of defect is suppressed. Thus, we expect that replica QMC measurements of topological EE will be a fundamental technique in the characterization of non-trivial topological phases in the future.

This work has been supported by the Natural Sciences and Engineering Research Council of Canada (NSERC), NSF grant No PHY 05-51164 (KITP) and the Swiss
FIG. 3: (a) The topological entanglement entropy (EE) measured on an $L = 8$ system as a function of inverse temperature $\beta = t/T$. The plateaus are a measure of the total quantum dimension $\sqrt{2}$, and should be $\ln(2)$ and $2\ln(2)$ for a $Z_2$ spin liquid. (b) The approach of the topological EE to the first plateau, for different system sizes. The value of the crossover temperature ($\beta_c$), measured at $2\gamma = \ln(2)/2$, shows a logarithmic dependence on system size (inset).
term from a cylindrical geometry without corners as in [21] we might find a different result. One interesting possibility is studying a system on the Klein bottle, which also has Euler characteristic zero and hence does not require defects in the lattice. The $Z_2$ theories have the same degeneracies on the Klein bottle but other theories may have different degeneracy.