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Entanglement entropy of critical spin liquids

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Quantum spin liquids are phases of matter whose internal structure is not captured by a local order parameter. Particularly intriguing are critical spin liquids, where strongly interacting excitations control low energy properties. Here we calculate their bipartite entanglement entropy that characterize their quantum structure. In particular we calculate the Renyi entropy S_2 , on model wavefunctions obtained by Gutzwiller projection of a Fermi sea. Although the wavefunctions are not sign positive, S_2 can be calculated on relatively large systems (>324 spins), using the variational Monte Carlo technique. On the triangular lattice we find that entanglement entropy of the projected Fermi-sea state violates the boundary law, with S_2 enhanced by a logarithmic factor. This is an unusual result for a bosonic wave-function reflecting the presence of emergent fermions. These techniques can be extended to study a wide class of other phases.

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Entanglement properties of a ground state wavefunction can serve as a diagnostic for characterizing a phase of matter [1]. Such a characterization is especially useful when a phase does not break any symmetry and consequently does not offer a local order parameter. Two examples of this observation are the presence of a non-zero topological entanglement entropy in a fully gapped topological ordered state [2] and the relation between the edge state spectrum and the entanglement spectrum for the quantum Hall states [3]. Entanglement thus encodes fundamental properties of a quantum phase, and intersects diverse fields including quantum information, many body physics and high energy theory [1].

Critical spin-liquids are a distinct class of states that also do not have a local order parameter. These gapless states are less well understood compared to the gapped spin-liquids which have topological order. Interestingly though, a large class of experiments suggest that they may well have been already realized in certain organic materials [4], which are quantum antiferromagnets on the triangular lattice. To gain a deeper understanding of these phases, in this paper we investigate the quantum structure of a class of critical spin-liquids from an information theoretic point of view. We demonstrate that entanglement properties of model ground states can be calculated, even on fairly large systems involving > 324 spins. In contrast to quantum Monte Carlo[5], we deal with non-positive wavefunctions that potentially describe ground states of frustrated quantum magnets.

Both gapped as well as gapless spin-liquids may be obtained within a slave-particle approach [6], where one expresses the spin operator in terms of a product of operators (f), denoting emergent particles : $\vec{S} = f_{\sigma}^{\dagger} \frac{\vec{\sigma}_{aa'}}{2} f_{\sigma'}$. In a spin liquid phases, these emergent particles are the appropriate low energy excitations. Inevitably, they appear coupled to gauge fields. Gapped spin liquids are described by topological quantum field theories and are relatively well understood. In contrast, spin-liquids with gapless, strongly interacting excitations (critical spin liq-

uids), are described by matter-gauge theories which are harder to analyze [7].

A critical spin liquid, the spinon fermi sea (SFS) state, has been invoked [8] to account for the intriguing phenomenology of aforementioned triangular lattice organic compounds [4]. In the SFS state, the f particles hop on the triangular lattice sites giving rise to a Fermi sea, while strongly interacting with an emergent ‘electromagnetic’ $U(1)$ gauge field. The metal like specific heat and thermal conductivity seen in these materials is potentially an indication of the spinon Fermi surface. A candidate ground state spin wavefunction for the SFS state suggested by the slave-particle formalism, is obtained by projecting out all doubly occupied states from the Fermi sea wavefunction. This Gutzwiller projection technique works well in one dimension. There, the projected Fermi sea spin wavefunction captures long distance properties of the Heisenberg chain, and is even the exact ground state of the Haldane-Sastry [9] Hamiltonian. Similar rigorous results are not available in two dimensions. However, the Gutzwiller projected Fermi sea is known to have excellent variational energy for the $J_2 - J_4$ spin model on the triangular lattice, which is believed to be appropriate for the forementioned triangular lattice compounds[8]. Detailed comparisons between the projected wavefunction and exact numerics have also been made[10].

Using the Variational Monte-Carlo technique, we calculate the bipartite entanglement entropy, in particular Renyi entropy S_2 of a critical spin liquid - the conjectured spinon Fermi sea state on the triangular lattice. We find a violation of the boundary law, with S_2 enhanced by a logarithmic factor, an unusual result for a bosonic wavefunction strongly suggesting the presence of emergent fermions with a Fermi surface. This is also consistent with the recent exact numerical studies on multi-leg ladder spin-1/2 ring exchange models where the central charge is found to increase in proportion to the number of legs [10]. We also calculate Renyi entropy for an algebraic spin liquid state [6, 11] obtained by Gutzwiller

projecting the wave function of free Fermions on a π flux square lattice. This state is found to obey the area law, consistent with the presence of emergent Dirac fermions in the system. Finally, we calculate Renyi entropy for projected Fermi sea state on the square lattice. Here a nested Fermi sea is present before projection. In this case the projection is found to result in long range magnetic order (see also [12]) and a significant reduction in entanglement entropy, especially of the area law violating term, compared to the unprojected Fermi gas. These different trends are found to set in even at relatively small system sizes, suggesting that this probe may be applied in the context of exact diagonalization and DMRG.

Renyi Entanglement Entropy: Given a normalized wavefunction, $|\phi\rangle$, and a partition of the system into subsystems A and B , one can trace out the subsystem B to give a density matrix on A : $\rho_A = \text{Tr}_B |\phi\rangle\langle\phi|$. The Renyi entropies are defined by:

$$S_n = \frac{1}{1-n} \log(\text{Tr} \rho_A^n) \quad (1)$$

It is common to pay special attention to the von Neumann entropy, $S_1 = -\text{Tr}[\rho_A \log \rho_A]$ (obtained by taking the limit $n \rightarrow 1$). However, the Renyi entropies seem equally good measures of entanglement as they share many properties with von Neumann entropy S_1 . Here we will focus on $S_2 = -\log(\text{Tr} \rho_A^2)$. For ground states of local Hamiltonians, both S_1 and S_2 are expected to follow a boundary law, i.e. they only grow as the surface area of the boundary of region A [1]. A well known violation occurs for critical phases in 1D, where in contrast to a constant as expected from the area law, $S_1, S_2 \sim \log L_A$, where L_A is the size of system A embedded inside an infinite line [13]. In higher dimensions, $D = 2, 3$ an area law is believed to hold for S_1, S_2 even for gapless states such as ordered phases with goldstone modes, and quantum critical points [5, 14, 15]. Both S_1, S_2 violate the area law in higher dimensions for free fermions with a Fermi surface [16, 17] and also share identical topological entanglement entropies for gapped phases [18]. Therefore S_2 seems as good a measure of physical properties as the von Neumann entropy, and is often easier to calculate [5] as we detail now for our problem. Furthermore we note the inequality $S_1 \geq S_2$. This will be important when we find violation of area law for S_2 as this would imply area law violation for the von Neumann entropy S_1 as well.

Monte Carlo Evaluation: Consider the wavefunction $\phi(a, b)$, where a (b) be the configuration of subsystem A (B). The Renyi entropy S_2 is conveniently expressed by imagining two copies of the system. Construct the product wavefunction: $|\Phi\rangle = \sum_{a,b,a',b'} \phi(a, b) \phi(a', b') |a, b\rangle |a', b'\rangle$, and define the Swap_A operator [5], which swaps the configurations of the A subsystem in the two copies: $\text{Swap}_A |a, b\rangle |a', b'\rangle = |a', b\rangle |a, b'\rangle$ then it is easily shown:

$$e^{-S_2} = \frac{\langle \Phi | \text{Swap}_A | \Phi \rangle}{\langle \Phi | \Phi \rangle} \quad (2)$$

This can be rewritten in a form suitable for Monte Carlo evaluation. Defining configurations $\alpha_1 = a, b, \alpha_2 = a', b'$ and $\beta_1 = a', b, \beta_2 = a, b'$,

$$\langle \text{Swap}_A \rangle = \sum_{\alpha_1 \alpha_2} \rho_{\alpha_1} \rho_{\alpha_2} f(\alpha_1, \alpha_2) \quad (3)$$

Here $f(\alpha_1, \alpha_2) = \frac{\phi_{\beta_1} \phi_{\beta_2}}{\phi_{\alpha_1} \phi_{\alpha_2}}$ is averaged by sampling with the normalized weights $\rho_{\alpha_i} = |\phi_{\alpha_i}|^2 / \sum_{\alpha_i} |\phi_{\alpha_i}|^2$

The Gutzwiller projected wavefunctions we will consider can be written as products of determinants. Such wavefunctions can be efficiently evaluated, which forms the basis for Variational Monte Carlo technique [19]. Since the entanglement entropy is at the very least expected to scale as the length of the boundary of subsystem A , $\sim L_A$, $\langle \text{Swap}_A \rangle$ is at least exponentially small in L_A . Evaluating this small quantity may pose a problem - one solution called the ‘ratio trick’ discussed in Ref [5] in the valence bond basis unfortunately does not work in our case, since the relevant states do not always have non-vanishing overlap unlike in that basis.

A more serious problem arises from the fact that $f(\alpha_1, \alpha_2)$ is not necessarily positive, for the wavefunctions we will study. This is in contrast to Quantum Monte Carlo studies with positive ground state wavefunctions [5]. With time reversal symmetry, $f(\alpha_1, \alpha_2)$ is real but can fluctuate in sign. The calculational effort for $\langle \text{Swap}_A \rangle$ is then found to scale exponentially with L_A . Although Variational Monte Carlo schemes are generally free of the fermionic sign problem, we encounter a mild variant here. Below we partially mitigate this by introducing a ‘sign trick’ algorithm that separates Swap_A into a product of two factors, both calculable within Variational Monte Carlo. This renders the calculation doable within few percent error for boundary sizes $L_A \lesssim 10$. For positive wavefunctions (i.e. ones that obey Marshall sign) we find an immense simplification, and the calculational cost only scales polynomially with L_A as in conventional Variational Monte Carlo. For a fixed value of boundary L_A , the cost of computation always scales polynomially with the total system size L irrespective of the wavefunction.

Sign Trick: After some algebra [20], Eqn.2 can in general be rewritten as a product of two averages:

$$\begin{aligned} \langle \text{Swap}_A \rangle &= \sum_{\alpha_1 \alpha_2} \rho_{\alpha_1} \rho_{\alpha_2} |f(\alpha_1, \alpha_2)| \left[\sum_{\alpha_1 \alpha_2} \tilde{\rho}_{\alpha_1, \alpha_2} e^{i\phi(\alpha_1, \alpha_2)} \right] \\ &= \langle \text{Swap}_{A, \text{mod}} \rangle \langle \text{Swap}_{A, \text{sign}} \rangle \end{aligned}$$

For real wavefunctions, the phase factor reduces to a sign. Empirically, we find this leads to significant gains,

the advantages are detailed in [20]. We benchmarked our algorithm for three free fermion tight binding problems on: 1) A one dimensional chain of $L = 200$ sites with L_A up to 100 sites, 2) An 18×18 square lattice with the linear size L_A up to 7 sites. 3) A honeycomb (graphene) lattice with Dirac dispersion. We find very good agreement with the exact results [20] that were calculated using the correlation matrix technique [21].

Gutzwiller Projected Spin Liquid Wavefunctions: Next we calculate Renyi entropy for the problems of our actual interest namely projected Fermi liquid wave functions which are considered good ansatz for ground states of critical spin-liquids. We analyze two different classes of critical spin-liquids: states that at the slave-particle mean-field level have a full Fermi surface of spinons and those with only nodal fermions. For a triangular lattice with uniform hopping $t_{rr'} = t$ one obtains a Fermi surface of spinons at the mean-field level while for a square-lattice with π flux through every plaquette (i.e. $\Pi_{\square} t_{rr'} = -1$) one obtains nodal Dirac fermions. We also study the projected wave function on square lattice with uniform hopping (and no flux).

The wave-functions for these spin-liquids are constructed by starting with a system of spin-1/2 fermionic spinons $f_{r\alpha}$ hopping on a finite lattice of size $L_1 \times L_2$ at half-filling with a mean field Hamiltonian: $H_{MF} = \sum_{rr'} [-t_{rr'} f_{r\sigma}^\dagger f_{r'\sigma} + h.c.]$. The spin wave-function is given by $|\phi\rangle = P_G |\phi\rangle_{MF}$ where $|\phi\rangle_{MF}$ is the ground state of H_{MF} and the Gutzwiller projector $P_G = \prod_i (1 - n_{i\uparrow} n_{i\downarrow})$ ensures exactly one fermion per site. The sign-structure of the projected wave-function depends markedly on the underlying lattice. For a bipartite lattice with $t_{rr'}$ non-zero and real only for the opposite sublattices, one can prove that the wave-function satisfies the Marshall sign rule [20]. Thus, for a bipartite lattice, one only needs to calculate $\langle \text{Swap}_{A,mod} \rangle$ since $\langle \text{Swap}_{A,sign} \rangle$ trivially equals unity. The projected wave-function for the square lattice with and without π -flux (as well as that for the one-dimensional Haldane-Shastry state) satisfies the Marshall's sign rule while that for the triangular lattice doesn't. We discuss these three cases separately. The one dimensional case was previously discussed in [22].

Triangular lattice: As mentioned above the mean-field ansatz describes a spin-liquid with spinons hopping on a triangular lattice. We consider a lattice with total size 18×18 on a torus and the region A of square geometry with linear size L_A upto 8 sites. We find a clear signature of $L_A \log L_A$ scaling in Renyi entropy (Fig. 1). This is rather striking since the wave-function is a spin wave-function and therefore could also be written in terms of hard-core bosons. This result strongly suggests the presence of an underlying spinon Fermi surface. In fact the coefficient of the $L_A \log L_A$ term is rather similar before and after projection. This observation may be rationalized by picturing a two dimensional Fermi surface as a collection of many independent one dimensional systems

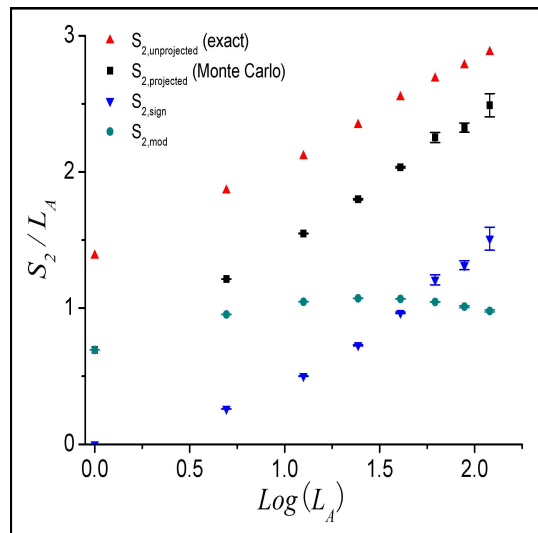


FIG. 1: Renyi entropy data for projected and unprojected Fermi sea state on the triangular lattice of size 18×18 with $L_A = 1 \dots 8$. Note, projection barely modifies the slope, pointing to a Fermi surface surviving in the spin wavefunction. We also separately plot $S_{2,sign}$ and $S_{2,mod}$ (as defined in the text) for the projected state, the former dominates at larger sizes.

in momentum space, each giving rise to a $\log L$ contribution. Gutzwiller projection then just removes a single charge degree of freedom.

It is interesting to compare the contribution to S_2 from $S_{2,sign} \equiv -\log(\langle \text{Swap}_{A,sign} \rangle)$ and $S_{2,mod} \equiv -\log(\langle \text{Swap}_{A,mod} \rangle)$ separately. Numerically, $S_{2,sign}$ appears to be responsible for the logarithmic violation of the area law (Fig. 1). This suggests that the sign structure of the wavefunction is crucial at least in this case.

The area-law violation of the Renyi entropy for Gutzwiller projected wave-functions substantiates the theoretical expectation that an underlying Fermi surface is present in the spin wavefunction.

Square lattice with π flux: The mean-field ansatz consists of spinons with Dirac dispersion around two nodes, say, $(\pi/2, \pi/2)$ and $(\pi/2, -\pi/2)$ (the locations of the nodes depend on the gauge one uses to enforce the π flux). The projected wave-function has been proposed in the past as the ground state of an algebraic spin liquid. The algebraic spin-liquid is believed to be describable by a strongly coupled conformal field theory of Dirac spinons coupled to a non-compact $SU(2)$ gauge field [6, 11]. Because of this the algebraic spin-liquid has algebraically decaying spin-spin correlations. We verify this explicitly for the projected wavefunction using Variational Monte Carlo on a 36×36 lattice [20]. This state is different from that in Ref. [23], where Majorana fermions are coupled to a discrete Z_2 gauge field making them effectively free at low energies, in contrast to our critical state.

Square lattice being bipartite, the projected wavefunc-

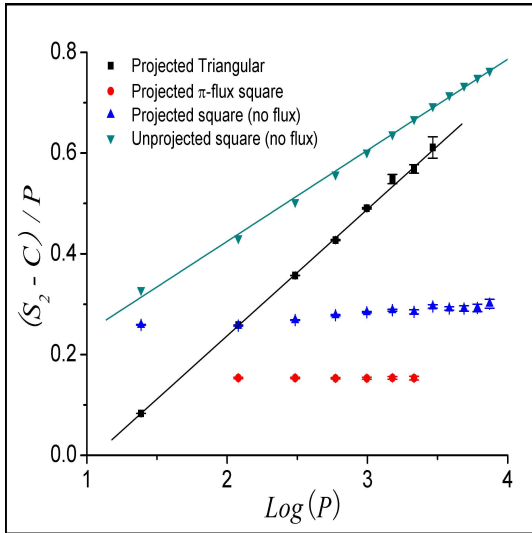


FIG. 2: Renyi entropy for the projected Fermi sea state on the triangular lattice and square (with and without π -flux) lattice as a function of the perimeter P of the subsystem A . Here C is the constant part of the S_2 . We find $S_2 \sim P \log(P) + C$ for the projected triangular lattice state while $S_2 \sim P + C$ for the projected π -flux square lattice state. For the square lattice state (no flux), the projection leads to a significant reduction in S_2 suggesting at most a very weak violation of the area-law.

tion satisfies Marshall's sign rule and hence we were able to perform Monte Carlo calculation of Renyi entropy on bigger lattice sizes compared to the triangular lattice case. We chose the overall geometry as a torus of size $L_A \times 4L_A$ with both region A and its complement of sizes $L_A \times 2L_A$ (the total boundary size being $L_A + L_A = 2L_A$). We considered L_A upto 14 sites. We found that the projected wavefunction follows an area law akin to its unprojected counterpart and has the scaling $S_2 \approx 0.30L_A + g$ where $g \approx 1.13$ is a universal constant that depends only on the aspect ratio of the geometry [15]. This is consistent with the presence of Dirac fermions at low energies.

Square lattice without any flux: The unprojected Fermi surface is nested. Since projection amounts to taking correlations into account, one might wonder whether the Fermi surface undergoes a magnetic instability after the projection. Indeed, we found non-zero magnetic order in the projected wave-function, consistent with an independent recent study Ref. [12]. This was verified by calculating spin-spin correlations on a 42×42 lattice [20]. Renyi entropy calculations were done on a lattice of total size 24×24 with region A being a square upto size 12×12 . The results are shown in the Fig. 2. Though it is difficult to rule out presence of a partial Fermi surface from Renyi entropy, there is a significant reduction in the Renyi entropy as well as the coefficient of $L_A \log L_A$ term as compared to the unprojected Fermi sea.

Summary: In this paper we described a route to calculating the Renyi entropy S_2 for a wide variety of wave-

functions that can be handled by the Variational Monte Carlo method. Our starting point is the ground state wave-function rather than the Hamiltonian. This allows us to study interesting states on relatively large systems, that may not be obtainable from sign problem free Hamiltonians. We calculated S_2 for Gutzwiller projected states that have been conjectured as the ground state wave-functions for gapless spin-liquids. We found that the projected Fermi sea on the triangular lattice violates the area law strongly indicating the presence of an emergent Fermi surface of neutral fermions. The sign structure of the wave-function makes a dominant contribution to the entropy. We note our algorithm is readily generalizable to calculate the higher Renyi entropies S_n ($n > 2$). Also, it can be applied to study partially projected Fermi sea wave-function which model correlated Fermi liquids. This opens a window to study the entanglement entropy of fermions away from the free limit. A very interesting direction that we leave for the future, is testing the Widom conjecture, proposed currently for free fermions[16], to interacting states with Fermi surfaces.

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