Entanglement, subsystem particle numbers and topology in free fermion systems

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Abstract

We study the relationship between bipartite entanglement, subsystem particle number and topology in a half-filled free fermion system. It is proposed that the spin-projected particle numbers can distinguish the quantum spin Hall state from other states, and can be used to establish a new topological index for the system. Furthermore, we apply the new topological invariant to a disordered system and show that a topological phase transition occurs when the disorder strength is increased beyond a critical value. It is also shown that the subsystem particle number fluctuation displays behavior very similar to that of the entanglement entropy. This provides a lower-bound estimation for the entanglement entropy, which can be utilized to obtain an estimate of the entanglement entropy experimentally.

Keywords: entanglement, subsystem particle number, topology, entanglement entropy

(Some figures may appear in colour only in the online journal)

1. Introduction

Topological phases of matter are usually distinguished by using some global topological properties, such as topological invariants and topologically protected gapless edge modes, rather than certain local order parameters. The integer quantum Hall effect [1], fractional quantum Hall effect [2], and band Chern insulators [3] can be characterized by Chern numbers or Berry phases [4, 5]. The quantum spin Hall (QSH) effect [6, 7] and the three-dimensional topological insulators [8, 9] are characterized by the $Z_2$ invariant [10] or spin Chern number [11, 12]. In recent years, quantum entanglement [13], which reveals the phase information of the quantum-mechanical ground-state wavefunction, has been used as a tool to characterize the topological phases. As shown by Levin and Wen [14] and also by Kitaev and Preskill [15], the existence of topological entanglement entropy in a fully gapped system, such as the fractional quantum Hall [17] and the gapped $Z_2$ spin liquid [14, 16] ones, indicates the existence of long-range quantum entanglement (topological order [18] in equivalent parlance). Interestingly, a very recent work [19] proved that topological order can also be read and assessed via the geometric entanglement in multipartite entangled systems. Further important progress is the demonstration that the entanglement spectrum (ES) [20] reveals the gapless edge spectrum for fractional quantum Hall systems [20–24], Chern insulators [25, 26], topological insulators [27–29] and even spin systems [30–32].

Supposing A and B to be two blocks of a large system in a pure quantum state, the reduced density matrix (RDM) $\rho_A$ can be obtained by tracing over the degrees of freedom of B. Then the Von Neumann entanglement entropy (EE) can be computed:

$$S_{\text{ent}} = -\text{Tr}(\rho_A \ln \rho_A) = -\text{Tr}(\rho_B \ln \rho_B).$$

(1)

It has been shown that for bipartite subsystems A and B with a smooth boundary, $S_{\text{ent}}$ has the form of $S_{\text{ent}} = \alpha L - S_{\text{top}}$, where $L$ is the length of the boundary, $\alpha$ is a non-universal coefficient and $-S_{\text{top}}$ is a universal constant called the topological entanglement entropy [14, 15]. Moreover, if we write the RDM in the form of $\rho_A = \exp(-H_{\text{ent}})/Z$, where $Z$ is a normalization constant and $H_{\text{ent}}$ is known as the entanglement Hamiltonian, the eigenvalue spectrum $\{\varepsilon_i\}$ of $H_{\text{ent}}$ is called the ES, which...
stores more information about the quantum entanglement than the EE [20].

In this paper, we study the relationship between bipartite entanglement and subsystem particle number in half-filled free fermion systems. It was proposed in [33], for systems with translational invariance in one dimension, that the discontinuity in the subsystem particle number as a function of the conserved momentum indicates whether or not the ES has a spectral flow, which is determined by the topological invariant of the system [29]. Nevertheless, this approach has an exceptional case for a half-filled QSH system with two-dimensional inversion symmetry. To overcome the inadequacy, we define spin-projected particle numbers, based on which spin trace indices can be well defined, for the QSH system with or without \( s_z \) conservation. Spin trace indices are unequivocally related to the topological invariant of the QSH system, i.e., the \( \mathbb{Z}_2 \) index. Furthermore, we show that spin trace indices will still work well in disordered systems and can demonstrate a topological phase transition. We further investigate the relationship between the EE and subsystem particle number fluctuation. The latter is also dominated by the boundary excitations of the system, and satisfies a similar area law to the EE.

In the next section, we introduce the model Hamiltonian, and explain the procedure for calculating the ES and EE. In section 3, numerical calculation of the ES is carried out, and the connection between the subsystem spin-projected particle numbers and the topological invariants in different phases is established. In section 4, we apply spin trace indices to a disordered system and show that it can demonstrate the phase transition from the QSH to the trivial insulator. In section 5, the relationship between the EE and subsystem particle number fluctuation is discussed. Our results are summarized and discussed in section 6.

2. The model Hamiltonian

We begin with the tight-binding model Hamiltonian for the QSH system introduced by Kane and Mele [6, 10], plus an additional exchange field [36]:

\[
H = -\sum_{\langle i,j \rangle} c^\dagger_i c_j + i v_{so} \sum_{\langle i,j \rangle} c^\dagger_i \sigma_z v_{ij} c_j + i v_r \sum_{\langle i,j \rangle} c^\dagger_i (\sigma \times d_{ij}) c_j + \sum_i m_i c^\dagger_i c_i + g \sum_i c^\dagger_i \sigma_z c_i. \tag{2}
\]

Here, the first term is the usual nearest neighbor hopping term with \( c^\dagger_i = (c^\dagger_i, c^\dagger_{i+}) \) as the electron creation operator on site \( i \), where the hopping integral is set to be unity. The second term is the intrinsic spin–orbit coupling (SOC) with coupling strength \( v_{so} \), where \( \langle i,j \rangle \) stand for the second-nearest neighbor sites, and \( v_{ij} = (di_{kj} \times dD_{kl})/\|di_{kj} \times dD_{kl}\| \). Here, \( k \) is the common nearest neighbor of \( i \) and \( j \), and vector \( di_{kj} \) points from \( i \) to \( j \). \( v_{ij} = +1 \) for counterclockwise hopping and \( v_{ij} = -1 \) otherwise. \( \sigma_z \) is a Pauli matrix describing the electron’s spin. The intrinsic SOC opens a band gap and drives the system into the QSH phase. The third term stands for the nearest neighbor Rashba SOC with \( \sigma \) the Pauli matrix and \( V_r \) the Rashba SOC strength. The intrinsic SOC term breaks the \( SU(2) \) symmetry down to \( U(1) \), and the Rashba SOC term breaks the remaining \( U(1) \) spin symmetry down to \( \mathbb{Z}_2 \). The fourth term stands for a staggered sublattice potential \( m_i = \pm m \), which also opens a gap at the Dirac point but drives the system into a trivial topology phase. The last term represents a uniform exchange field with strength \( g \), which explicitly violates the time reversal symmetry.

We consider systems with cylinder or torus boundary conditions, consisting of \( N_y \) (\( N_x \) to be even) zigzag chains along the circumferential direction (\( y \) direction). The size of the sample will be denoted as \( N = N_x \times N_y \), with \( N_y \) the number of atomic sites on each chain. We take the entanglement cut along the \( y \) direction, which results in one or two interfaces between the two equal parts A and B, respectively, for the cylinder or torus geometry, as shown in figure 1. In order to examine the EE and ES, a Schmidt decomposition of the ground-state wavefunction or calculation of the RDM is usually needed. For non-interacting fermion systems, however, the necessary information of the entanglement can also be obtained from the following two-point correlators [37]:

\[
c_{\tau_1,\tau_2}(i,j) = \langle c^\dagger_{\tau_1}(i) c_{\tau_2}(j) \rangle. \tag{3}
\]

Here, \( \langle \cdot \rangle \) means the ground-state expectation of an operator. \( \tau \) can be an index of a spin, pseudospin or orbital degree of freedom.

Using the Fourier transformation (FT) along the \( y \) direction, the Hamiltonian can be rewritten as follows:

\[
H = \sum_{k_i,i,j} c^\dagger_i(k_y) h_{i,j}(k_y) c_j(k_y), \quad \text{where} \quad c^\dagger_i(k_y) = (c^\dagger_{i,\uparrow}(k_y), c^\dagger_{i,\downarrow}(k_y)), \quad c_{i,\sigma}(k_y) \text{ are the electron creation operators.}
\]

After performing the entanglement cut, we treat part \( A \) as the subsystem, and trace out the degrees of freedom of \( B \). It should be noted that all of the correlators \( c_{\tau_1,\tau_2}(i,j) \) with \( i \) and \( j \) confined in \( A \) are unchanged by the tracing. When carrying out the FT on the correlators, we can get

\[
c_{\tau_1,\tau_2}(i,j) = \frac{1}{N_y} \sum_{k_y} e^{ik_y(i-j)} \langle c^\dagger_{\tau_1}(k_y) c_{\tau_2}(k_y) \rangle, \tag{4}
\]

where \( i \) and \( j \) discriminate between the zigzag chains. We use \( \langle c^\dagger_{\tau_1}(k_y)c_{\tau_2}(k_y) \rangle \) to form a Hermitian matrix \( C(k_y) \). Then the entanglement Hamiltonian is given by [37]

\[
H_{\text{ent}} = \ln(C^{-1} - 1). \tag{5}
\]
The spectrum \( \{ \varepsilon_i \} \) of \( \mathcal{C} \) is related to the spectrum \( \{ \varepsilon_i \} \) of \( H_{\text{tot}} \) by \( \varepsilon_i = 1/(e^\varepsilon_i + 1) \), where \( \varepsilon_i \) acts as the average fermion number in the entanglement energy level \( \varepsilon_i \) at ‘temperature’ \( T = 1 \). By using the spectrum of \( \mathcal{C} \), the EE at each \( k_y \) sector is given by \( s_{\text{ent}}(k_y) = \sum_i s_i \), with

\[
s_i = -\varepsilon_i \ln \varepsilon_i - (1 - \varepsilon_i) \ln(1 - \varepsilon_i).
\]

From the viewpoint of probability theory, \( s_i \) in equation (6) can be regarded as the Shannon (information) entropy of the Bernoulli distribution, i.e., the \( i \)th entanglement level \( \varepsilon_i \) has the probability \( \varepsilon_i \) of being occupied while it has the probability \( 1 - \varepsilon_i \) of being unoccupied. As a result, \( S_{\text{ent}} \) is the Shannon entropy of a series of such independent Bernoulli distributions. In the following, we will perform systematic numerical simulations to study various phases of Hamiltonian (2) in terms of the ES and the subsystem particle number.

3. The entanglement spectrum and subsystem particle number

At \( g = 0 \), Hamiltonian (2) is the standard Kane–Mele model [6], which is invariant under time reversal symmetry. The system is in a QSH phase when \( |m/v_{\text{so}}| < |9 - \frac{1}{4}(v_g/v_{\text{so}})^2| \), and is an insulator when \( |m/v_{\text{so}}| > |9 - \frac{1}{4}(v_g/v_{\text{so}})^2| \). On the other hand, if we set \( v_{\text{so}} = 0 \), \( v_g \) and \( g \) nonzero, a middle band gap opens when \( |g| \neq |m| \). The system is in a quantum anomalous Hall phase with Chern number \( C = \pm 2 \) [36] for \( |g| < |m| \), and is an insulator for \( |g| > |m| \). The band gap closes at the transition point \( |g| = |m| \). The phase diagram for \( v_{\text{so}} = 0 \) and \( v_g \neq 0 \) is plotted in figure 2(g).

Figures 2(a) and (b) show the ES for the QSH phase, figures 2(c) and (d) for the insulator phase and figures 2(e) and (f) for the quantum anomalous Hall phase. Here, it should be emphasized that the nontrivial topological phases exhibit gapless ES (figures 2(a), (b), (e) and (f)), corresponding to physical gapless edge modes, and this property is named the spectral flow [29], which has been explained by Qi and co-workers for coupled conformally invariant subsystems with left- and right-moving particles in all chiral topological systems [26]. However, the spectral flow is broken for the topologically trivial phase (figures 2(c) and (d)), which is also consistent with the property of the corresponding edge states.

In a recent work [33], the authors proposed a new characteristic quantity called the ‘trace index’ for describing topological invariants, which is defined through a subsystem particle number operator \( N_A(k_y) = \sum_{i \in A} \xi_i^c \xi_i^c \). The expectation of \( N_A(k_y) \) is given by

\[
\langle N_A(k_y) \rangle = \langle GS | \sum_{i \in A} \xi_i^c(k_y) \xi_i(k_y) | GS \rangle = \text{Tr} \mathcal{C}.
\]

In figure 3, we plot the expectation of \( N_A(k_y) \) for the three different phases mentioned above. In the cylinder geometry, \( N_A(k_y) \) is discontinuous at some discrete momenta in the nontrivial topological phases, as shown in figures 3(a) and (c). This is in contrast to the case for the normal insulator phase (see figure 3(b)), where \( N_A(k_y) \) is a continuous function of \( k_y \). In the torus geometry, \( N_A(k_y) \) is exactly equal to half of...
the total particle number in the $k_y$ sector, without showing any discontinuity, because the change of the particle number in $A$ around interface 1 is just canceled by that around interface II due to the rotation invariance of the torus. In the cylinder geometry, the trace index was defined as the total of the discontinuities of $\langle N_A(k_y) \rangle$ with varying momentum. Alexandradinata, Hughes and Bernevig [33] presented a detailed analysis and proved that the trace index is equivalent to the Chern number (or $Z_2$ invariant) for the Chern ($Z_2$) insulators.

Therefore, the subsystem particle number provides a new alternative tool for revealing the topological invariants.

However, as mentioned in [33], there is an exceptional case in which the subspace of the occupied bands at the symmetric momenta is not closed under time reversal in the ground state. If at the symmetric momenta the Kramers doublet that extends along the edge of $A$ is singly occupied, $\langle N_A(k_y) \rangle$ is continuous, even when the system is in a nontrivial topological phase. For the half-filled system under consideration, the topological invariants.

The spin-projected subsystem particle numbers $C_{\alpha}$, are related to $\{\alpha\}$ for the QSH phase (figures 4(a)–(c)) and $Z_2$ mod 2, which labels the topologically distinct phases.

We plot $Tr \, C^{\alpha}$ ($\alpha = \pm$) as functions of $k_y$ in figure 4. No matter whether $s_z$ is conserved or not, both $Tr \, C^{+}(k_y)$ and $Tr \, C^{-}(k_y)$ show discontinuities at $k_y = \pi$ with $A^+ = 1$ and $A^- = -1$ in the QSH phase (figures 4(a) and (b)), where the two-dimensional inversion symmetry is present ($m = 0$). Figure 4(c) shows the discontinuities of $Tr \, C^{+}(k_y)$ and $Tr \, C^{-}(k_y)$ in the QSH phase in which $s_z$ is not conserved ($\nu_r \neq 0$) and the two-dimensional inversion symmetry is broken ($m \neq 0$). In this case, the spin trace indices are equal to 1 and $-1$, respectively, contributed by two different momentum points. But, in contrast, both $Tr \, C^{+}(k_y)$ and $Tr \, C^{-}(k_y)$ are continuous functions in the normal insulator phase (figure 4(d)). Consequently, it is easy to get $A_{Z_2} = 1$ for the QSH phase (figures 4(a)–(c)) and $A_{Z_2} = 0$ for the insulator phase (figure 4(d)). Therefore, the subsystem particle number expectation can be used to characterize the topological invariants. In particular, for the QSH systems, the spin trace indices are well-defined quantities that can reveal the $Z_2$ invariant and distinguish different quantum phases.
on-site potential of the form
\[ \sum \text{disorder effect}, \]
we include into Hamiltonian (2) a random properties and, in particular, to say something about the localization to topological phases, but it will be equally important to extract disordered system sample sizes.

averaged over 400 disorder configurations, for several different one time disorder configuration with disorder strength parameter \( W \) as a function of the disorder strength parameter \( W \).

\[ W_\text{c} \approx 5.2 \] should become a sudden drop from \( \pm 1 \) to 0 in the thermodynamic limit. In short, as long as disorder is present, loss of translational invariance leads to a loss of the Brillouin zone, and consequently the \( Z_2 \) index cannot be defined, so how one abstracts the topological invariant from disordered systems becomes very significant. Here the (disordered) spin trace indices that we have defined above can be applied to these systems and can display a topological phase transition occurring when the disorder strength is increased beyond a critical value.

\[ \Delta N_A^2(k_y) = \langle N_A^2(k_y) \rangle - \langle N_A(k_y) \rangle^2. \] (12)

Substituting equation (7) into (12) and using Wick’s theorem to expand all four-point correlators, one can obtain

\[ \Delta N_A^2(k_y) = \sum_{i,j \in A} (c_{i,k_y}^\dagger c_{j,k_y}^\dagger c_{j,k_y} c_{i,k_y}) \]

yielding \( \Delta N_A^2(k_y) = \sum \xi_i (1 - \xi_i) \), which is in keeping with the variance formula of the Bernoulli distributions. In order to find a definite relationship between the EE and the variance, one can construct a concave function \( f(x) = -\ln x/(1-x) \) for \( x \in [0,1] \), and apply Jensen’s inequality

\[ -x \ln x - (1-x) \ln(1-x) \geq (4 \ln 2)x(1-x). \] (14)
verify

1

eliminated by adiabatic continuous deformation, which may
particle number fluctuation and the EE, which cannot be
topology phases contributes a maximal value to the subsystem
entangled state with
lately [40], and here we find that the similarity persists for the
one. This similarity was observed in non-topological systems
somewhat similarly, and are very close to the corresponding EE
all cases, the curves for the particle number fluctuation behave
directly proportional to the particle number fluctuation of the
of the EE is given by
proof. From the inequality, one can see that a lower bound
and here, as a complement, we give a very simple and direct

Figure 6. Entanglement entropy in comparison with subsystem
particle number fluctuation for (a), (b) the QSH phase, (c), (d)
the insulator phase and ((e), (f)) the quantum anomalous Hall phase,
in the cylinder geometry (left panels) and in the torus geometry
(right panels). All the parameters are the same as in figure 2.

The equality holds if and only if $x = 1/2$. Equation (14)
enables us to give a lower-bound estimation of the EE:

\[ s_{\text{ent}}(k_y) \geq (4 \ln 2) \Delta N_{\Lambda}^2(k_y). \]  (15)

This inequality is first given in the context of metal [39]
and here, as a complement, we give a very simple and direct
proof. From the inequality, one can see that a lower bound of the EE is given by $s_0(k_y) \equiv (4 \ln 2) \cdot \Delta N_{\Lambda}^2(k_y)$, which is
directly proportional to the particle number fluctuation of the
subsystem. In figure 6, we plot $s_{\text{ent}}(k_y)$ and $s_0(k_y)$ for the QSH
phase, insulator phase and quantum anomalous Hall phase. In
all cases, the curves for the particle number fluctuation behave
somewhat similarly, and are very close to the corresponding EE
one. This similarity was observed in non-topological systems
lately [40], and here we find that the similarity persists for the
topologically nontrivial system. Moreover, each maximally
entangled state with $\epsilon_m = 0$ ($\epsilon_m = 1/2$) existing only in
topology phases contributes a maximal value to the subsystem
number fluctuation and the EE, which cannot be
eliminated by adiabatic continuous deformation, which may
provide a new way for probing topological insulators.

Furthermore, one can use $N_{\Lambda}(k_y) = \sum_{i \in A} \epsilon_i^k \gamma_i^k$ to
verify $\Delta N_{\Lambda}^2 = \sum_{k_y} \Delta N_{\Lambda}^2(k_y) \rightarrow \frac{L_y}{2\pi} \int \text{d} k_y \Delta N_{\Lambda}^2(k_y)$, indicating
that $\Delta N_{\Lambda}^2(k_y)$ satisfies an area law [38], similar to that
for the EE: $s_{\text{ent}} = \sum_{k_y} s_{\text{ent}}(k_y) \rightarrow \frac{L_y}{2\pi} \int \text{d} k_y s_{\text{ent}}(k_y)$. Remarkably, for
topologically ordered states, [19] proved that the non-topologically ordered term of the geometric entanglement obeys a similar area law in multipartite entanglement. We ex-
pect that the conclusion should still be true for non-interacting
fermion systems. To conclude, the subsystem particle number
fluctuation shares several common characteristics with the
EE, and so can be utilized to obtain an estimate of the EE.
The EE has been widely used in analyzing quantum critical
phenomena, topologically ordered states and evolution after a
quantum quench, as well as quantum computation [44].

6. Summary and discussion

To conclude, we have investigated the relationship between
the quantum entanglement and subsystem particle number.
The spin trace indices can reveal the topological invariants
and be used to classify different phases in QSH systems.
This new tool always works well even though $s_c$ is not
conserved. Even in a disordered system, it works well and
can be used to demonstrate a topological phase transition. As
for the subsystem particle number fluctuation, it shares several
common properties with the EE. They satisfy the same area
law and are dominated by the boundary excitations with each zero mode having a maximal contribution. The connection
between the two quantities is universal, regardless of whether or not the system has a nontrivial band topology. As a result,
the subsystem particle number fluctuation, as an observable
quantity, can be utilized to obtain an estimate of the EE
experimentally [40].

As long as the Fermi energy lies in the bulk energy gap, all results that we have obtained will remain about the
same. With the Fermi energy lowered into the valence band
or increased into the conduction band, the spin trace indices
will no longer be quantized and will continuously drop from $\pm 1$ to 0. We also stress that the results obtained in this paper
only hold for free fermion systems. Interestingly, as regards
the entanglement entropy and the subsystem particle number
fluctuation, a similar relation has been found for certain kinds
of interacting systems, for example, one-dimensional quantum
spin chains [41], although such a relation does not hold true for some other interacting systems such as fractional
quantum Hall states [42] and the two-dimensional spin-1/2
antiferromagnetic Heisenberg model [43].

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